# Geometric Analysis of the Metropolis Algorithm in Lipschitz Domain

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# Geometric Analysis for the Metropolis Algorithm on Lipschitz Domains


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**Abstract**

This paper gives geometric tools: comparison, Nash and Sobolev inequalities for pieces of the relevent Markov operators, that give useful bounds on rates of convergence for the Metropolis algorithm. As an example, we treat the random placement of $N$ hard discs in the unit square, the original application of the Metropolis algorithm.


## 1 Introduction and Results

Let $\Omega$ be a bounded, connected open subset of $\mathbb{R}^d$. We assume that its boundary, $\partial\Omega$, has Lipschitz regularity. Let $B_1$ be the unit ball of $\mathbb{R}^d$ and $\varphi(z) = \frac{1}{\mathrm{vol}(B_1)} 1_{B_1}(z)$ so that $\int \varphi(z)dz = 1$. Let $\rho(x)$ be a measurable positive bounded function on $\overline{\Omega}$ such that $\int_\Omega \rho(x)dx = 1$. For $h \in ]0,1]$, set

$$K_{h,\rho}(x,y) = h^{-d}\varphi\left(\frac{x-y}{h}\right)\min\left(\frac{\rho(y)}{\rho(x)}, 1\right), \tag{1.1}$$

and let $T_{h,\rho}$ be the Metropolis operator associated with these data, that is,

$$\begin{aligned} T_{h,\rho}(u)(x) &= m_{h,\rho}(x)u(x) + \int_\Omega K_{h,\rho}(x,y)u(y)dy, \\ m_{h,\rho}(x) &= 1 - \int_\Omega K_{h,\rho}(x,y)dy \geq 0. \end{aligned} \tag{1.2}$$

Then the Metropolis kernel $T_{h,\rho}(x,dy) = m_{h,\rho}(x)\delta_{x=y} + K_{h,\rho}(x,y)dy$ is a Markov kernel, the operator $T_{h,\rho}$ is self-adjoint on $L^2(\Omega, \rho(x)dx)$, and thus the probability measure $\rho(x)dx$ on $\Omega$ is


*Supported in part by the National Science Foundation, DMS 0505673.

†Supported in part by ANR equa-disp Blan07-3-188618



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§Supported in part by ANR equa-disp Blan07-3-188618

stationary. For $n \geq 1$, we denote by $T^n_{h,\rho}(x, dy)$ the kernel of the iterated operator $(T_{h,\rho})^n$. For any $x \in \Omega$, $T^n_{h,\rho}(x, dy)$ is a probability measure on $\Omega$, and our main goal is to get some estimates on the rate of convergence, when $n \to +\infty$, of the probability $T^n_{h,\rho}(x, dy)$ toward the stationary probability $\rho(y)dy$.

A good example to keep in mind is the random placement of $N$ non-overlapping discs of radius $\varepsilon > 0$ in the unit square. This was the original motivation for the work of Metropolis et al. [MRR+53]. One version of their algorithm goes as follows: from a feasable configuration, pick a disc (uniformly at random) and a point within distance $h$ of the center of the chosen disc (uniformly at random). If recentering the chosen disc at the chosen point results in a feasable configuration, the change is made. Otherwise, the configuration is kept as it started. If $N$ is fixed and $\varepsilon$ and $h$ are small, this gives a Markov chain with a uniform stationary distribution over all feasable configurations. The state space consists of the $N$ centers corresponding to feasible configurations. It is a bounded domain with a Lipschitz boundary when $N\epsilon$ is small (see Section 4, Proposition 4.1). The scientific motivation for the study of random packing of hard discs as a way of understanding the apparent existence of a liquid/solid phase transition for arbitrarily large temperatures (for suitably large pressure) is clearly described in Uhlenbeck [Uhl68, Sect. 5, p. 18]. An overview of the large literature is in Lowen [Löw00]. Entry to the zoo of modern algorithms to do the simulation (particularly in the dense case) with many examples is in Krauth [Kra06]. Further discussion, showing that the problem is still of current interest, is in Radin [Rad08].

We shall denote by $g(h, \rho)$ the spectral gap of the Metropolis operator $T_{h,\rho}$. It is defined as the largest constant such that the following inequality holds true for all $u \in L^2(\rho) = L^2(\Omega, \rho(x)dx)$.

$$\|u\|^2_{L^2(\rho)} - (u|1)^2_{L^2(\rho)} \leq \frac{1}{g(h,\rho)}(u - T_{h,\rho}u|u)_{L^2(\rho)}, \tag{1.3}$$

or equivalently,

$$\int_{\Omega\times\Omega} |u(x) - u(y)|^2 \rho(x)\rho(y)dxdy \leq \frac{1}{g(h,\rho)} \int_{\Omega\times\Omega} K_{h,\rho}(x, y)|u(x) - u(y)|^2 \rho(x)dxdy. \tag{1.4}$$

**Definition 1.** We say that an open set $\Omega \subset \mathbb{R}^d$ is Lipschitz if it is bounded and for all $a \in \partial\Omega$ there exists an orthonormal basis $\mathcal{R}_a$ of $\mathbb{R}^d$, an open set $V = V'\times ]-\alpha, \alpha[$ and a Lipschitz map $\eta : V' \to ]-\alpha, \alpha[$ such that in the coordinates of $\mathcal{R}_a$, we have

$$\begin{aligned} V \cap \Omega &= \left\{ \left(y', y_d < \eta(y')\right), (y', y_d) \in V'\times ]-\alpha, \alpha[ \right\} \\ V \cap \partial\Omega &= \left\{ \left(y', \eta(y')\right), y' \in V' \right\}. \end{aligned} \tag{1.5}$$

Our first result is the following:

**Theorem 1.1.** *Let $\Omega$ be an open, connected, bounded, Lipschitz subset of $\mathbb{R}^d$. Let $0 < m \leq M < \infty$ be given numbers. There exists $h_0 > 0$, $\delta_0 \in ]0, 1/2[$ and constants $C_i > 0$ such that for any $h \in ]0, h_0]$, and any probability density $\rho$ on $\Omega$ which satisfies for all $x$, $m \leq \rho(x) \leq M$, the following holds true.*

*i) The spectrum of $T_{h,\rho}$ is a subset of $[-1+\delta_0, 1]$, $1$ is a simple eigenvalue of $T_{h,\rho}$, and $\mathrm{Spec}(T_{h,\rho}) \cap [1 - \delta_0, 1]$ is discrete. Moreover, for any $0 \leq \lambda \leq \delta_0 h^{-2}$, the number of eigenvalues of $T_{h,\rho}$ in $[1 - h^2\lambda, 1]$ (with multiplicity) is bounded by $C_1(1 + \lambda)^{d/2}$.*

*ii) The spectral gap $g(h, \rho)$ satisfies*

$$C_2h^2 \leq g(h, \rho) \leq C_3h^2 \tag{1.6}$$

*and the following estimate holds true for all integer n:*

$$sup_{x\in\Omega}\|T^n_{h,\rho}(x,dy)-\rho(y)dy\|_{TV}\le C_4e^{-ng(h,\rho)}. \tag{1.7}$$

The next result will give some more information on the behavior of the spectral gap $g(h,\rho)$ when $h\to 0$. To state this result, let

$$\alpha_d=\int\varphi(z)z_1^2dz=\frac{1}{d}\int\varphi(z)|z|^2dz=\frac{1}{d+2} \tag{1.8}$$

and let us define $\nu(\rho)$ as the largest constant such that the following inequality holds true for all $u$ in the Sobolev space $H^1(\Omega)$:

$$\|u\|^2_{L^2(\rho)}-(u|1)^2_{L^2(\rho)}\le\frac{1}{\nu(\rho)}\frac{\alpha_d}{2}\int_\Omega|\nabla u|^2(x)\rho(x)dx, \tag{1.9}$$

or equivalently,

$$\int_{\Omega\times\Omega}|u(x)-u(y)|^2\rho(x)\rho(y)dxdy\le\frac{\alpha_d}{\nu(\rho)}\int_\Omega|\nabla u|^2(x)\rho(x)dx. \tag{1.10}$$

Observe that for a Lipschitz domain $\Omega$, the constant $\nu(\rho)$ is well-defined thanks to Sobolev embedding. For a smooth density $\rho$, this number $\nu(\rho)>0$ is closely related to the unbounded operator $L_\rho$ acting on on $L^2(\rho)$.

$$\begin{aligned}L_\rho(u)&=\frac{-\alpha_d}{2}(\triangle u+\frac{\nabla\rho}{\rho}.\nabla u)\\ D(L_\rho)&=\left\{u\in H^1(\Omega),-\Delta u\in L^2(\Omega),\partial_n u|_{\partial\Omega}=0\right\}\end{aligned} \tag{1.11}$$

We now justify and explain the choice of domain in (1.11). Background for the following discussion and tools for working in Lipschitz domains is in [AF03].

When $\Omega$ has smooth boundary, standard elliptic regularity results show that for any $u\in H^1(\Omega)$ such that $-\Delta u\in L^2(\Omega)$, the normal derivative of $u$ at the boundary, $\partial_n u=\overrightarrow{n}(x).\nabla u|_{\partial\Omega}$ is well defined and belongs to the Sobolev space $H^{-1/2}(\partial\Omega)$. Here, we denote by $\overrightarrow{n}(x)$ the incoming unit normal vector to $\partial\Omega$ at a point $x$. In the case where $\partial\Omega$ has only Lipschitz regularity, the Sobolev spaces $H^s(\partial\Omega)$ are well defined for all $s\in[-1,1]$. The trace operator, $\gamma_0(u)=u|_{\partial\Omega}$ maps $H^1(\Omega)$ onto $H^{1/2}(\partial\Omega)=Ran(\gamma_0)$, and its kernel is $Ker(\gamma_0)=H^1_0(\Omega)$. Equipped with the norm $\|u\|_{H^{1/2}}=\inf\{\|v\|_{H^1},\ \gamma_0(v)=u\}$ it is an Hilbert space. Then, for any $\varphi\in H^{1/2}(\partial\Omega)^*$, there exists a unique $v\in H^{-1/2}(\partial\Omega)$ such that $\varphi(u)=\int_{\partial\Omega}vud\sigma$ for all $u\in H^{1/2}(\partial\Omega)$ (where $\sigma$ is the measure induced on the boundary). For $v\in H^{-1/2}(\partial\Omega)$, the support of $v$ can be defined in a standard way. The trace operator acting on vector fields $u\in(L^2)^d$ with $\mathrm{div}(u)\in L^2$,

$$\gamma_1:\left\{u\in(L^2(\Omega))^d,\mathrm{div}(u)\in L^2(\Omega)\right\}\to H^{-1/2}(\partial\Omega), \tag{1.12}$$

is then defined by the formula

$$\int_\Omega\mathrm{div}(u)(x)v(x)dx=-\int_\Omega u(x).\nabla v(x)dx-\int_{\partial\Omega}\gamma_1(u)v|_{\partial\Omega}d\sigma(x),\ \forall v\in H^1(\Omega). \tag{1.13}$$

In particular, for $u\in H^1(\Omega)$ satisfying $\Delta u=\mathrm{div}\nabla u\in L^2(\Omega)$ we can define $\partial_n u|_{\partial\Omega}=\gamma_1(\nabla u)\in H^{-1/2}(\partial\Omega)$ and the set $D(L_\rho)$ is well defined. From (1.13) we deduce that for any $u\in H^1(\Omega)$ with $\Delta u\in L^2$ and any $v\in H^1(\Omega)$ we have

$$\langle(L_\rho+1)u,v\rangle_{L^2(\rho)}=\frac{\alpha_d}{2}\left(\langle\nabla u,\nabla v\rangle_{L^2(\rho)}+\langle\partial_n u,\rho v\rangle_{H^{-1/2}(\partial\Omega),H^{1/2}(\partial\Omega)}\right)+\langle u,v\rangle_{L^2(\rho)}. \tag{1.14}$$

Then, it is standard that $L_\rho$ is the self-adjoint realization of the Dirichlet form

$$\frac{\alpha_d}{2}\int_\Omega |\nabla u(x)|^2\rho(x)dx. \tag{1.15}$$

A standard argument [RS78, Sects. 13, 14] using Sobolev embedding show that $L_\rho$ has a compact resolvant. Denote its spectrum by $\nu_0 = 0 < \nu_1 < \nu_2 < \dots$ and by $m_j$ the multiplicity of $\nu_j$. In particular, $\nu(\rho) = \nu_1$. Observe also that $m_0 = 1$ since $KerL$ is spanned by the constant function equal to 1.

To state our theorem, we need a basic definition:

**Definition 2.** Let $\Omega$ be a Lipschitz open set of $\mathbb{R}^d$. We say that $\partial\Omega$ is quasi-regular if $\partial\Omega = \Gamma_{\text{reg}} \cup \Gamma_{\text{sing}}, \Gamma_{\text{reg}} \cap \Gamma_{\text{sing}} = \emptyset$ with $\Gamma_{\text{reg}}$ a finite union of smooth hypersurfaces, relatively open in $\partial\Omega$, and $\Gamma_{\text{sing}}$ a closed subset of $\mathbb{R}^d$ such that

$$v \in H^{-1/2}(\partial\Omega) \quad \textit{and} \quad \sup(v) \subset \Gamma_{\text{sing}} \Longrightarrow v = 0. \tag{1.16}$$

Observe that 1.16 is obviously satisfied if $\partial\Omega$ is smooth, since in that case one can take $\Gamma_{\text{sing}} = \emptyset$. More generally, the boundary is quasi-regular if it is 'piece-wise smooth' in the following sense: suppose $\Omega$ is a Lipschitz open set of $\mathbb{R}^d$ such that $\partial\Omega = \Gamma_{\text{reg}} \cup \Gamma_{\text{sing}},\ \Gamma_{\text{reg}} \cap \Gamma_{\text{sing}} = \emptyset$, where $\Gamma_{\text{reg}}$ is a smooth hypersurface of $\mathbb{R}^d$, relatively open in $\partial\Omega$, and $\Gamma_{\text{sing}}$ a closed subset of $\mathbb{R}^d$ such that $\Gamma_{\text{sing}} = \cup_{j\geq 2} S_j$ where the $S_j$ are smooth disjoint submanifolds of $\mathbb{R}^d$ such that

$$\text{codim}_{\mathbb{R}^d} S_j \geq j, \qquad \cup_{k\geq j} S_k = \overline{S_j}, \tag{1.17}$$

then $\Omega$ is quasi-regular, since in that case, if $v \in H^{-1/2}(\partial\Omega)$ is such that near a point $x_0$, the support of $v$ is contained in a submanifold $S$ of codimension $\geq 2$ in $\mathbb{R}^d$, then $v = 0$ near $x_0$. This follows from the fact that the distribution $\langle u, \phi\rangle = \langle v, \phi|_{\partial\Omega}\rangle$ on $\mathbb{R}^d$ belongs to $H^{-1}(\mathbb{R}^d)$, and if $u \in \mathcal{D}'(\mathbb{R}^d)$ is such that $u \in H^{-1}(\mathbb{R}^d)$ and $\sup(u) \subset \{x_1 = x_2 = 0\}$, then $u = 0$. As an example, a cube in $\mathbb{R}^d$ is quasi-regular. This 'piece-wise smooth' condition (often called "stratified") is easy to visualize. In our applications (Section 4) it was hard to work with products of stratified sets. The definition we give works easily with products and is exactly what is needed in the proof.

**Theorem 1.2.** *Let $\Omega$ be an open, connected, bounded and Lipschitz subset of $\mathbb{R}^d$, such that $\partial\Omega$ is quasi-regular. Assume that the positive density $\rho$ is continuous on $\overline{\Omega}$. Then*

$$\lim_{h\to 0} h^{-2} g(h, \rho) = \nu(\rho). \tag{1.18}$$

*Moreover, if the density $\rho$ is smooth on $\overline{\Omega}$, then for any $R > 0$ and $\varepsilon > 0$ such that $\nu_{j+1} - \nu_j > 2\varepsilon$ for $\nu_{j+2} < R$, there exists $h_1 > 0$ such that one has for all $h \in ]0, h_1]$,*

$$\text{Spec}\left(\frac{1 - T_{h,\rho}}{h^2}\right) \cap ]0, R] \subset \cup_{j\geq 1}[\nu_j - \varepsilon, \nu_j + \varepsilon], \tag{1.19}$$

*and the number of eigenvalues of $\frac{1-T_{h,\rho}}{h^2}$ in the interval $[\nu_j - \varepsilon, \nu_j + \varepsilon]$ is equal to $m_j$.*

Theorem 1.1 is proved in Section 2. This is done from the spectrum of the operator by comparison with a 'ball walk' on a big box $B$ containing $\Omega$. One novelty is the use of 'normal extensions' of functions from $\Omega$ to $B$ allowing comparison of the two Dirichlet forms. When the Dirichlet forms and stationary distributions for random walk on a compact group are comparible, the rates of convergence are comparable as well [DSC93, Lemma 5]. Here, the Metropolis Markov chain is far from a random walk on a group. Indeed, because of the holding implicit in the Metropolis algorithm, the operator does not have any smoothing properties. The transfer of information is carried out by a Sobolev inequality for a spectrally-truncated part of the operator. This is transfered to a Nash inequality and then an inductive argument is used to obtain decay bounds on iterates of the kernel. A further technique is the use of crude Weyl type estimates to get bounds on the number of eigenvalues close to 1. All of these enter the proof of the total variation estimate (1.7). All of these techniques seem broadly applicable.

Theorem 1.2 is proved in Section 3. It gives rigorous underpinnings to a general picture of the spectrum of the Metropolis algorithm based on small steps. This was observed and proved in special cases [DL08], [LM08]. The picture is this: because of the holding (or presence of the multiplier $m_{h,\rho}$ in (1.2)) in the Metropolis algorithm, the operator always has continuous spectrum. This is well isolated from 1 and can be neglected in bounding rates of convergence. The spectrum near 1 is discrete and for $h$ small, merges with the spectrum of an associated Neumann problem. This is an analytic version of the weak convergence of the discrete time Metropolis chain to the Langevin diffusion with generator (1.11).

In Section 4, we return to the hard disc problem showing that a suitable power of the operators and domains involved satisfies our hypothesis. Precisely, in Theorem 4.6 we shall prove that the results of Theorem 1.1 and Theorem 1.2 hold true in this case.

## 2 A Proof of Theorem 1.1

Let us recall that

$$K_{h,\rho}(x,y) = h^{-d}\varphi\left(\frac{x-y}{h}\right)\min\left(\frac{\rho(y)}{\rho(x)},1\right), \tag{2.1}$$

so that

$$\begin{aligned} T_{h,\rho}(u) &= u - Q_{h,\rho}(u), \\ Q_{h,\rho}(u)(x) &= \int_\Omega K_{h,\rho}(x,y)\,(u(x)-u(y))\,dy, \\ ((1-T_{h,\rho})u|u)_{L^2(\rho)} &= \frac{1}{2}\int\int_{\Omega\times\Omega}|u(x)-u(y)|^2 K_{h,\rho}(x,y)\rho(x)dxdy. \end{aligned} \tag{2.2}$$

Observe that since $\Omega$ is Lipschitz, from (1.2) we get that for any $h_0>0$, there exists $\delta_0>0$ such that for any density $\rho$ with $0\le m\le\rho(x)\le M$ one has $sup_{x\in\Omega}m_{h,\rho}(x)\le 1-2\delta_0$ for all $h\in]0,h_0]$. Thus the essential spectrum of $T_h$ is a subset of $[0,1-2\delta_0]$ and the spectrum of $T_h$ in $[1-\delta_0,1]$ is discrete. From the last line of 2.2, we get that if $u\in L^2$ is such that $u=T_{h,\rho}(u)$, then $u(x)=u(y)$ for almost all $x,y\in\Omega, |x-y|<h$ and since $\Omega$ is connected, $u$ is constant. Therefore, 1 is a simple eigenvalue of $T_{h,\rho}$. In particular, for any $h>0$, the spectral gap satisfies

$$g(h,\rho)>0 \tag{2.3}$$

For the proof of Theorem 1.1, we will not really care about the precise choice of the density $\rho$. In fact, if $\rho_1,\rho_2$ are two densities such that $m\le\rho_i(x)\le M$ for all $x$, then

$$\begin{aligned} \rho_2(x) &\le \rho_1(x)\left(1+\frac{\|\rho_1-\rho_2\|_\infty}{m}\right), \\ K_{h,\rho_1}(x,y)\rho_1(x) &\le K_{h,\rho_2}(x,y)\rho_2(x)\left(1+\frac{\|\rho_1-\rho_2\|_\infty}{m}\right), \end{aligned} \tag{2.4}$$

and this implies, using the definition (1.4) of the spectral gap and of $\nu_\rho$,

$$
\begin{aligned}
\frac{g_{h,\rho_1}}{g_{h,\rho_2}} &\leq \left(1+\frac{\|\rho_1-\rho_2\|_\infty}{m}\right)^3, \\
\frac{\nu_{\rho_1}}{\nu_{\rho_2}} &\leq \left(1+\frac{\|\rho_1-\rho_2\|_\infty}{m}\right)^3.
\end{aligned} \tag{2.5}
$$

In particular, it is sufficient to prove (1.6) for a constant density.

The proof that for some $\delta_0 > 0$, independent of $\rho$, one has $\mathrm{Spec}(T_{h,\rho}) \subset [-1+\delta_0, 1]$ for all $h \in ]0, h_0]$ is the following: one has

$$
(u + T_{h,\rho}u|u)_{L^2(\rho)} = \frac{1}{2}\int_{\Omega\times\Omega} K_{h,\rho}(x,y)|u(x)+u(y)|^2\rho(x)dxdy + 2(m_{h,\rho}u|u)_{L^2(\rho)}. \tag{2.6}
$$

Therefore, it is sufficient to prove that there exists $h_0, C_0 > 0$ such that the following inequality holds true for all $h \in ]0, h_0]$ and all $u \in L^2(\Omega)$:

$$
\int_{\Omega\times\Omega} h^{-d}\varphi\left(\frac{x-y}{h}\right)|u(x)+u(y)|^2dxdy \geq C_0\|u\|^2_{L^2(\Omega)}. \tag{2.7}
$$

Let $\omega_j \subset \Omega$, $\cup_j\omega_j = \Omega$ be a covering of $\Omega$ such that $\mathrm{diam}(\omega_j) < h$ and for some $C_i > 0$ independent of $h$, $\mathrm{vol}(\omega_j) \geq C_1h^d$, and for any $j$, the number of $k$ such that $\omega_j \cap \omega_k \neq \emptyset$ is less than $C_2$. Such a covering exists as $\Omega$ is Lipschitz. Then

$$
\begin{aligned}
C_2\int_{\Omega\times\Omega} h^{-d}\varphi\left(\frac{x-y}{h}\right)|u(x)+u(y)|^2dxdy &\geq \sum_j\int_{\omega_j\times\omega_j} h^{-d}\varphi\left(\frac{x-y}{h}\right)|u(x)+u(y)|^2dxdy \\
&\geq \sum_j h^{-d}\frac{1}{|B_1|}\int_{\omega_j\times\omega_j}|u(x)+u(y)|^2dxdy \\
&\geq \sum_j 2h^{-d}\frac{1}{|B_1|}\mathrm{vol}(\omega_j)\|u\|^2_{L^2(\omega_j)} \\
&\geq \frac{2C_1}{|B_1|}\|u\|^2_{L^2(\Omega)}.
\end{aligned} \tag{2.8}
$$

From (2.8), we get that (2.7) holds true.

For the proof of (1.6) we need a suitable covering of $\Omega$. Given $\epsilon > 0$ small enough, there exists some open sets $\Omega_0, \dots, \Omega_N$ such that $\{x \in \mathbb{R}^d, \mathrm{dist}(x, \overline{\Omega}) \leq \epsilon^2\} \subset \cup_{j=0}^N\Omega_j$, where the $\Omega_j$'s have the following properties:

1. $\Omega_0 = \{x \in \Omega, d(x, \partial\Omega) > \epsilon^2\}$.

2. For $j = 1, \dots, N$, there exists $r_j > 0$, an affine isometry $R_j$ of $\mathbb{R}^d$ and a Lipschitz map $\varphi_j : \mathbb{R}^{d-1} \to \mathbb{R}$ such that, denoting $\tilde{\phi}_j(x', x_d) = (x', x_d + \varphi_j(x'))$ and $\phi_j = R_j \circ \tilde{\phi}_j$, we have

$$
\begin{aligned}
\phi_j &\text{ is injective on } B(0,2r_j)\times]-2\epsilon, 2\epsilon[ \\
\Omega_j &= \phi_j(B(0,r_j)\times]-\epsilon,\epsilon[) \\
\Omega_j\cap\Omega &= \phi_j(B(0,r_j)\times]0,\epsilon[) \\
\phi_j&\left(B(0,2r_j)\times]0,2\epsilon[\right) \subset \Omega
\end{aligned} \tag{2.9}
$$

We put our open set $\Omega$ in a large box $B = ]-A/2, A/2[^d$ and define an extension map $E : L^2(\Omega) \to L^2(B)$. For $j = 0, \dots, N$ we let $\chi_j \in C_0^\infty(\Omega_j)$ be such that $\sum_j \chi_j(x) = 1$ for $\operatorname{dist}(x, \overline{\Omega}) \leq \epsilon^2$. For any function $u \in L^2(\Omega)$, let $u_j, j = 0, \dots, N$ be defined in a neighborhood of $\Omega_j$ by $u_j = u \circ \phi_j \circ S \circ \phi_j^{-1}$, where $S(x', x_d) = (x', -x_d)$ if $x_d < 0$ and $S(x', x_d) = (x', x_d)$ if $x_d \geq 0$. For $x \in \Omega \cap \Omega_j$, one has $u_j(x) = u(x)$ and we define

$$E(u)(x) = \sum_{j=0}^{N} \chi_j(x) u_j(x). \tag{2.10}$$

We observe that $\tilde{\phi}_j^{-1}(x) = (x', x_d - \varphi_j(x'))$. Consequently, as $\varphi_j$ is Lipschitz-continuous, then $\phi_j$ and $\phi_j^{-1}$ are also Lipschitz-continuous. Hence, formula (2.10), gives us an extension map from $L^2(\Omega)$ into $L^2(B)$, which is also bounded from $H^1(\Omega)$ into $H^1(B)$. For $u \in L^2(\Omega), v \in L^2(B)$, set

$$\begin{aligned} \mathcal{E}_{h,\rho}(u) &= ((1 - T_{h,\rho})u|u)_{L^2(\rho)}, \\ \mathcal{E}_h(v) &= \int\int_{B \times B, |x-y| \leq h} h^{-d} |v(x) - v(y)|^2 dx dy. \end{aligned} \tag{2.11}$$

Since for $A$ large, $E(u)$ vanishes near the boundary of $B$, we can extend $v = E(u)$ as an $A$-periodic function on $\mathbb{R}^d$, and write its Fourier series $v(x) = E(u)(x) = \sum_{k \in \mathbb{Z}^d} c_k(v) e^{2i\pi kx/A}$ with $c_k(v) = A^{-d} \int_B e^{-2i\pi kx/A} v(x) dx$. Then

$$\begin{aligned} \|E(u)\|^2_{L^2(B)} &= A^d \sum_k |c_k|^2 \simeq \|u\|^2_{L^2(\Omega)}, \\ \|E(u)\|^2_{H^1(B)} &= A^d \sum_k (1 + 4\pi^2 k^2/A^2) |c_k|^2 \simeq \|u\|^2_{H^1(\Omega)}. \end{aligned} \tag{2.12}$$

Moreover, one gets

$$\begin{aligned} \mathcal{E}_h(v) &= A^d \sum_k |c_k|^2 \theta(hk), \\ \theta(\xi) &= \int_{|z| \leq 1} |e^{2i\pi \xi z/A} - 1|^2 dz. \end{aligned} \tag{2.13}$$

Observe that the function $\theta$ is nonnegative, quadratic near 0 and has a positive lower bound for $|\xi| \geq 1$.

The next two lemmas show that the Dirichlet forms for $u \in L^2(\Omega)$ and its extension to $L^2(B)$ are comparable.

**Lemma 2.1.** *For all $\alpha > 1$, there exists $C > 0$ and $h_0 > 0$ such that*

$$\mathcal{E}_{\alpha h,\rho}(u) \leq C \mathcal{E}_{h,\rho}(u) \qquad \forall u \in L^2(\Omega),\ \forall h \in ]0, h_0]. \tag{2.14}$$

*Proof.* Using (2.2) and (2.4), we observe that it suffices to prove the lemma in the case where $\rho(x) = \rho$ is constant, and we first we show the result when $\Omega$ is convex. In that case, since $|u(x) - u(y)| \leq |u(x) - u(\frac{x+y}{2})| + |u(\frac{x+y}{2}) - u(y)|$, one has

$$\begin{aligned} \mathcal{E}_{\alpha h,\rho}(u) &= \frac{(h\alpha)^{-d}}{2\operatorname{vol}(B_1)} \int_\Omega \int_\Omega 1_{|x-y| \leq \alpha h} |u(x) - u(y)|^2 \rho dx dy \\ &\leq \frac{2(h\alpha)^{-d}}{\operatorname{vol}(B_1)} \int_\Omega \int_\Omega 1_{|x-y| \leq \alpha h} |u(x) - u(\frac{x+y}{2})|^2 \rho dx dy \\ &= \frac{2(h\alpha/2)^{-d}}{\operatorname{vol}(B_1)} \int_{\phi(\Omega \times \Omega)} 1_{|x-y| \leq \frac{\alpha h}{2}} |u(x) - u(y)|^2 \rho dx dy, \end{aligned} \tag{2.15}$$

where $\phi(x,y) = (x, \frac{x+y}{2})$. As $\Omega$ is convex $\phi(\Omega\times\Omega) \subset \Omega\times\Omega$ and we get $\mathcal{E}_{\alpha h,\rho}(u) \leq 4\mathcal{E}_{\frac{\alpha h}{2},\rho}(u)$. Iterating this process we obtain the anounced result for convex domains.

In the general case, we use the local covering introduced in (2.9). Let $\Omega_i^+ = \Omega_i \cap \Omega$ (respectively $\Omega_i^- = \Omega_i \cap (\mathbb{R}^d \setminus \Omega)$) and $U_i(h) = \{(x,y) \in \Omega_i^+ \times \Omega, |x-y| \leq \alpha h\}$. Since by (2.2), $\Omega \subset \cup_i \Omega_i^+$, we have $\mathcal{E}_{\alpha h,\rho}(u) \leq \sum_{i=0}^N \mathcal{E}^i_{\alpha h,\rho}(u)$ with

$$\mathcal{E}^i_{\alpha h,\rho}(u) = \frac{(\alpha h)^{-d}}{2\mathrm{vol}(B_1)} \int_{U_i(h)} 1_{|x-y|\leq\alpha h} |u(x)-u(y)|^2 \rho dxdy. \tag{2.16}$$

Let us estimate $\mathcal{E}^0_{\alpha h,\rho}(u)$. For $h \in ]0, \epsilon^2/\alpha[$ and $(x,y) \in U_0(h)$, we have $[x,y] \subset \Omega$. Therefore, the change of variable $\phi(x,y) = (x, \frac{x+y}{2})$ maps $U_0(h)$ into $\Omega_0 \times \Omega$ and we get as above

$$\mathcal{E}^0_{\alpha h,\rho}(u) \leq \frac{2(\alpha h)^{-d}}{\mathrm{vol}(B_1)} \int_{U_0(h)} 1_{|x-y|\leq\alpha h} |u(x) - u(\frac{x+y}{2})|^2 \rho dxdy \leq 4\mathcal{E}_{\frac{\alpha h}{2},\rho}(u). \tag{2.17}$$

For $i \neq 0$ and $h > 0$ small enough, we remark that $U_i(h) \subset \tilde{\Omega}_i^+ \times \tilde{\Omega}_i^+$, where $\tilde{\Omega}_i^{\pm} = \phi_i(B(0,2r_i) \times \{0 < \pm x_d < 2\epsilon\})$. Denoting $Q_i = B(0,r_i) \times ]0,\epsilon[$, $\tilde{Q}_i = B(0,2r_i) \times ]0,2\epsilon[$, we can use the Lipschitz-continuous change of variable $\phi_i : \tilde{Q}_i \to \tilde{\Omega}_i^+ \subset \Omega$ to get

$$\mathcal{E}^i_{\alpha h,\rho}(u) \leq \frac{(\alpha h)^{-d}}{2\mathrm{vol}(B_1)} \int_{\tilde{Q}_i}\int_{\tilde{Q}_i} J_{\phi_i}(x) J_{\phi_i}(y) 1_{|\phi_i(x)-\phi_i(y)|\leq\alpha h} |u\circ\phi_i(x) - u\circ\phi_i(y)|^2 \rho dxdy \tag{2.18}$$

where the Jacobian $J_{\phi_i}$ of $\phi_i$ is a bounded function defined almost everywhere. As both $\phi_i, \phi_i^{-1}$ are Lipschitz-continuous, there exists $M_i, m_i > 0$ such that for all $x,y \in \tilde{Q}_i$ we have $m_i|x-y| \leq |\phi_i(x) - \phi_i(y)| \leq M_i|x-y|$. Therefore,

$$\mathcal{E}^i_{\alpha h,\rho}(u) \leq Ch^{-d} \int_{\tilde{Q}_i}\int_{\tilde{Q}_i} 1_{|x-y|\leq\frac{\alpha h}{m_i}} |u\circ\phi_i(x) - u\circ\phi_i(y)|^2 \rho dxdy, \tag{2.19}$$

where $C$ denotes a positive constant changing from line to line. As $\tilde{Q}_i$ is convex, it follows from the study of the convex case that

$$\begin{aligned}
\mathcal{E}^i_{\alpha h,\rho}(u) &\leq Ch^{-d} \int_{\tilde{Q}_i}\int_{\tilde{Q}_i} 1_{|x-y|\leq\frac{h}{M_i}} |u\circ\phi_i(x) - u\circ\phi_i(y)|^2 \rho dxdy \\
&\leq Ch^{-d} \int_{\tilde{Q}_i}\int_{\tilde{Q}_i} 1_{|\phi_i(x)-\phi_i(y)|\leq h} |u\circ\phi_i(x) - u\circ\phi_i(y)|^2 \rho dxdy \\
&\leq Ch^{-d} \int_{\tilde{\Omega}_i^+}\int_{\tilde{\Omega}_i^+} 1_{|x-y|\leq h} |u(x) - u(y)|^2 \rho dxdy \leq C_i \mathcal{E}_{h,\rho}(u),
\end{aligned} \tag{2.20}$$

and the proof is complete. □

**Lemma 2.2.** *There exist $C_0, h_0 > 0$ such that the following holds true for any $h \in ]0,h_0]$ and any $u \in L^2(\rho)$.*

$$\mathcal{E}_{h,\rho}(u)/C_0 \leq \mathcal{E}_h(E(u)) \leq C_0\left(\mathcal{E}_{h,\rho}(u) + h^2\|u\|^2_{L^2}\right). \tag{2.21}$$

*As a byproduct, there exists $C_1$ such that for all $h \in ]0,h_0]$, any function $u \in L^2(\rho)$ such that*

$$\|u\|^2_{L^2(\rho)} + h^{-2}\left((1-T_{h,\rho})u|u\right)_{L^2(\rho)} \leq 1$$

*admits a decomposition $u = u_L + u_H$ with $u_L \in H^1(\Omega)$, $\|u_L\|_{H^1} \leq C_1$, and $\|u_H\|_{L^2} \leq C_1 h$.*

*Proof.* Using the second line of (2.4), we may assume that the density $\rho$ is constant. The proof of the left inequality in (2.21) is obvious. For the upper bound, we remark that there exists $C > 0$ such that $\mathcal{E}_h(E(u)) \leq C \sum_{j=0}^{N} (\mathcal{E}_h^{j,1} + \mathcal{E}_h^{j,2})$ with

$$\mathcal{E}_h^{j,1} = h^{-d} \int_{B \times B} 1_{|x-y| \leq h} |\chi_j(x) - \chi_j(y)|^2 |u_j(x)|^2 dxdy \tag{2.22}$$

and

$$\mathcal{E}_h^{j,2} = h^{-d} \int_{B \times B} 1_{|x-y| \leq h} |\chi_j(y)|^2 |u_j(x) - u_j(y)|^2 dxdy. \tag{2.23}$$

As the functions $\chi_j$ are regular, there exist some $\tilde{\chi}_j \in C_0^\infty(B)$ equal to 1 near the support of $\chi_j$ such that

$$\mathcal{E}_h^{j,1} \leq C h^{-d} \int_B \tilde{\chi}_j(x) |u_j(x)|^2 \left( \int_B 1_{|x-y| \leq h} |x-y|^2 dy \right) dx \leq C h^2 \|u\|_{L^2(\Omega)}^2. \tag{2.24}$$

In order to estimate $\mathcal{E}_h^{j,2}$ one has to estimate the contribution of the points $x \in \Omega, y \notin \Omega$ and $x \notin \Omega, y \notin \Omega$. All the terms are treated in the same way and we only examine

$$\begin{aligned} \mathcal{E}_h^{j,3} &= h^{-d} \int_{\Omega \times (B \setminus \Omega)} 1_{|x-y| \leq h} |\chi_j(y)|^2 |u_j(x) - u_j(y)|^2 dxdy \\ &= h^{-d} \int_{\tilde{\Omega}_j^+ \times \Omega_j^-} 1_{|x-y| \leq h} |\chi_j(y)|^2 |u(x) - u \circ \phi_j \circ S \circ \phi_j^{-1}(y)|^2 dxdy, \end{aligned} \tag{2.25}$$

with $S$ defined below (2.9). Let $\sigma : \mathbb{R}^d \to \mathbb{R}^d$ be the symmetry with respect to $\{y_d = 0\}$, so that $S\sigma = Id$ on $\{y_d < 0\}$. We use the Lipschitz-continuous change of variable $\psi_j : y \in \Omega_j^+ \mapsto \phi_j \circ \sigma \circ \phi_j^{-1}(y) \in \Omega_j^-$ to get

$$\mathcal{E}_h^{j,3} \leq C h^{-d} \int_{\tilde{\Omega}_j^+ \times \Omega_j^+} 1_{|x-\psi_j(y)| \leq h} |\chi_j \circ \psi_j(y)|^2 |u(x) - u(y)|^2 dxdy. \tag{2.26}$$

We claim that there exists $\beta > 0$ such that

$$|\psi_j(y) - x| \geq \beta^{-1} |x-y| \qquad \forall (x,y) \in \tilde{\Omega}_j^+ \times \Omega_j^+. \tag{2.27}$$

Indeed, as both $\phi_j$ and $\phi_j^{-1}$ are Lipschitz-continuous, (2.27) is equivalent to finding $\beta > 0$ such that

$$|\sigma(y) - x| \geq \beta^{-1} |x-y| \qquad \forall (x,y) \in \phi_j^{-1}(\tilde{\Omega}_j^+ \times \Omega_j^+), \tag{2.28}$$

which is obvious with $\beta = 1$. From (2.27) it follows that for some $\alpha > 1$, one has

$$\mathcal{E}_h^{j,3} \leq C h^{-d} \int_{\tilde{\Omega}_j^+ \times \Omega_j^+} 1_{|x-y| \leq \alpha h} |u(z) - u(y)|^2 dzdy \leq C \mathcal{E}_{\alpha h, \rho}(u), \tag{2.29}$$

and the upper bound is then a straightforward consequence of Lemma 2.1.

The by-product is obtained by projecting the extension $v = E(u)$ on low frequencies $h|k| \leq 1$ and high frequencies $h|k| > 1$ and the fact that the function $\theta$ is quadratic near 0 and has a positive lower bound for $|\xi| \geq 1$. The proof of Lemma 2.2 is complete. $\square$

We are in position to prove the estimate (1.6) on the spectral gap. To show the right inequality, it suffices to plug a function $u \in C_0^\infty(\Omega)$ into (1.3) with support contained in a small ball $Q \subset \Omega$ and such that $\int_\Omega u(x)\rho(x)dx = 0$. As $Q$ is convex, it follows from Taylor's formula that for such $u$, we have $\langle u - T_h u, u\rangle = O(h^2)$.

To show the left inequality in (1.6), we first observe that it is clearly satisfied when $\Omega$ is convex. Indeed, given $u \in L^2(\Omega)$ we have by Cauchy-Schwarz

$$\int_{\Omega\times\Omega} |u(x)-u(y)|^2 dxdy \leq Ch^{-1} \sum_{k=0}^{K(h)-1} \int_{\Omega\times\Omega} |u\left(x+k\hbar(y-x)\right) - u\left(x+(k+1)\hbar(y-x)\right)|^2 dxdy, \tag{2.30}$$

where $K(h)$ is the greatest integer $\leq h^{-1}$ and $K(h)\hbar = 1$. With the new variables $x' = x+k\hbar(y-x)$, $y' = x+(k+1)\hbar(y-x)$, one has $dx'dy' = \hbar^d dxdy$ and we get

$$\int_{\Omega\times\Omega} |u(x)-u(y)|^2 dxdy \leq Ch^{-d-1}K(h)\int_{\Omega\times\Omega} 1_{|x'-y'|<\hbar \mathrm{diam}(\Omega)} |u(x')-u(y')|^2 dx'dy', \tag{2.31}$$

By lemma 2.1, this proves the left inequality in (1.6) in the case where $\Omega$ is convex.

In the general case, we can find some open sets contained in $\Omega$, $\omega_j \subset\subset \Omega_j^+ \subset\subset \tilde{\Omega}_j^+$, $j = 1,\dots,N+M$ such that for $j = 1,\dots,N$, $\Omega_j^+, \tilde{\Omega}_j^+$ are given in the previous lemma, $(\Omega_j^+)_{j=N+1,\dots,N+M}$ are convex $\Omega_0 \subset \cup_{j=N+1}^{M+N}\Omega_j^+$, $\Omega \subset \cup_{j=1}^{N+M}\omega_j$, and where $A \subset\subset B$ means that $\overline{A}^\Omega \subset B$. Hence for $h>0$ small enough,

$$\begin{aligned} \mathcal{E}_{h,\rho}(u) &\geq C\sum_{j=1}^{N+M} h^{-d}\int_{\Omega_j^+\times\tilde{\Omega}_j^+} 1_{|x-y|<h}(u(x)-u(y))^2 dxdy \\ &\geq C\sum_{j=1}^{N} h^{-d}\int_{Q_j\times\tilde{Q}_j} 1_{|\phi_j(x)-\phi_j(y)|<h}(u\circ\phi_j(x)-u\circ\phi_j(y))^2 dxdy \\ &\quad + C\sum_{j=N+1}^{N+M} h^{-d}\int_{\Omega_j^+\times\tilde{\Omega}_j^+} 1_{|x-y|<h}(u(x)-u(y))^2 dxdy. \end{aligned} \tag{2.32}$$

From the estimate proved precedently in the convex case, we know that there exists $a>0$ independant of $h$ such that the second sum in (2.32) is bounded from below by

$$Ch^2 \sum_{j=N+1}^{N+M}\int_{\omega_j\times\Omega_j^+} \left(u(x)-u(y)\right)^2 dxdy \geq Ch^2\sum_{j=N+1}^{N+M}\int_{\omega_j\times\Omega,|x-y|<a}\left(u(x)-u(y)\right)^2 dxdy. \tag{2.33}$$

On the other hand, thanks to the fact that $\phi_j$ is a Lipschitz diffeomorphism, there exists $\alpha>0$ such that $1_{|x-y|<h/\alpha} \leq 1_{|\phi_j(x)-\phi_j(y)|<h} \leq 1_{|x-y|<\alpha h}$. Using the convexity of $Q_i$ and Lemma 2.1 it follows that the first sum in the right hand side of (2.32) is bounded from below by

$$Ch^2\sum_{j=1}^{N}\int_{\omega_j\times\Omega,|x-y|<a}\left(u(x)-u(y)\right)^2 dxdy. \tag{2.34}$$

Combining (2.32), (2.33) and (2.34), we get

$$\mathcal{E}_{h,\rho}(u) \geq Ch^2\int_{\Omega\times\Omega,|x-y|<a}\left(u(x)-u(y)\right)^2 dxdy \tag{2.35}$$

for some fixed $a > 0$ independant of $h$. Since by (2.3) we have $g(a, \rho) > 0$, we get

$$\mathcal{E}_{h,\rho}(u) \geq Ch^2 \int_{\Omega\times\Omega} (u(x) - u(y))^2 \, dxdy \tag{2.36}$$

The proof of (1.6) is complete.

**Lemma 2.3.** *There exists $\delta_0 \in ]0, 1/2[$ such that* $\mathrm{Spec}(T_{h,\rho}) \cap [1 - \delta_0, 1]$ *is discrete, and for any $0 \leq \lambda \leq \delta_0/h^2$, the number of eigenvalues of $T_h$ in $[1 - h^2\lambda, 1]$ (with multiplicity) is bounded by $C_1(1 + \lambda)^{d/2}$. Moreover, any eigenfuntion $T_h(u) = \lambda u$ with $\lambda \in [1 - \delta_0, 1]$ satisfies the bound*

$$\|u\|_{L^\infty} \leq C_2 h^{-d/2} \|u\|_{L^2}. \tag{2.37}$$

*Proof.* To get (2.37), we just write that since $\lambda$ is not in the range of $m_h$, one has

$$u(x) = \frac{1}{\lambda - m_h(x)} \int_\Omega h^{-d} \varphi\left(\frac{x - y}{h}\right) \min\left(\frac{\rho(y)}{\rho(x)}, 1\right) u(y) dy,$$

and we apply Cauchy–Schwarz. The important point here is the estimate on the number of eigenvalues in $[1 - h^2\lambda, 1]$ by a power of $\lambda$. This is obtained by the min-max and uses (2.21). The min-max gives: if for some closed subspace $F$ of $L^2(\rho)$ with *codim*$(F) = N$ one has for all $u \in F$, $h^{-2}((1 - T_h)u|u)_{L^2(\rho)} \geq \lambda \|u\|^2_{L^2(\rho)}$, then the number of eigenvalues of $T_h$ in $[1 - h^2\lambda, 1]$ (with multiplicity) is bounded by $\mathrm{codim}(F) = N$. Then, we fix $c > 0$ small enough, and we choose for $F$ the subspace of functions $u$ such that their extension $v = E(u)$ is such that the Fourier coefficients satisfy $c_k(E(u)) = 0$ for $|k| \leq D$ with $hD \leq c$. The codimension of this space $F$ is exactly the number of $k \in \mathbb{Z}^d$ such that $|k| \leq D$, since if $p$ is a trigonometric polynomial such that $E^*(p) = 0$, we will have $\int_\Omega p(x)u(x)dx = 0$ for any function $u$ with compact support in $\Omega$ and such that $E(u) = u$, and this implies $p = 0$. Thus $\mathrm{codim}(F) \simeq (1 + D)^d$. On the other hand, the right inequality in (2.21) gives for $u \in F$, $h^{-2}((1 - T_h)u|u)_{L^2(\rho)} \geq C_0(D^2 - C_1)\|u\|^2_{L^2(\rho)}$ for universal $C_0, C_1$, since by (2.13), there exists $C > 0$ such that one has $\theta(hk)h^{-2} \geq CD^2$ for all $D \leq c/h$ and all $|k| > D$. The proof of our lemma is complete. □

We are now ready to prove the total variation estimate (1.7). We use the notation $T_h = T_{h,\rho}$ and $T^n_{h,x_0} = T^n_{h,\rho}(x_0, dy)$. Let $\Pi_0$ be the orthogonal projector in $L^2(f)$ on the space of constant functions

$$\Pi_0(u)(x) = 1_\Omega(x) \int_\Omega u(y)\rho(y)dy. \tag{2.38}$$

Then

$$2 \sup_{x_0\in\Omega} \|T^n_{h,x_0} - \rho(y)dy\|_{TV} = \|T^n_h - \Pi_0\|_{L^\infty\to L^\infty}. \tag{2.39}$$

Thus, we have to prove that there exist $C_0, h_0$, such that for any $n$ and any $h \in ]0, h_0]$, one has

$$\|T^n_h - \Pi_0\|_{L^\infty\to L^\infty} \leq C_0 e^{-ng_{h,\rho}}. \tag{2.40}$$

Observe that since we know that for $h_0$ small, the estimate (1.6) holds true for any $\rho$, we may assume $n \geq Ch^{-2}$. In order to prove (2.40), we split $T_h$ into three pieces, using spectral theory.

Let $0 < \lambda_{1,h} \leq \cdots \leq \lambda_{j,h} \leq \lambda_{j+1,h} \leq \cdots \leq h^{-2}\delta_0$ be such that the eigenvalues of $T_h$ in the interval $[1 - \delta_0, 1[$ are the $1 - h^2\lambda_{j,h}$, with associated orthonormal eigenfunctions $e_{j,h}$,

$$T_h(e_{j,h}) = (1 - h^2\lambda_{j,h})e_{j,h}, \qquad (e_{j,h}|e_{k,h})_{L^2(\rho)} = \delta_{j,k}. \tag{2.41}$$

Then we write $T_h - \Pi_0 = T_{h,1} + T_{h,2} + T_{h,3}$ with

$$\begin{aligned} T_{h,1}(x,y) &= \sum_{\lambda_{1,h} \le \lambda_{j,h} \le h^{-\alpha}} (1-h^2\lambda_{j,h}) e_{j,h}(x) e_{j,h}(y), \\ T_{h,2}(x,y) &= \sum_{h^{-\alpha} < \lambda_{j,h} \le h^{-2}\delta_0} (1-h^2\lambda_{j,h}) e_{j,h}(x) e_{j,h}(y), \\ T_{h,3} &= T_h - \Pi_0 - T_{h,1} - T_{h,2}. \end{aligned} \tag{2.42}$$

Here $\alpha > 0$ is a small constant that will be chosen later. One has $T_h^n - \Pi_0 = T_{h,1}^n + T_{h,2}^n + T_{h,3}^n$, and we will get the bound (2.40) for each of the three terms. We start by very rough bounds. Since there are at most $Ch^{-d}$ eigenvalues $\lambda_{j,h}$ and using the bound (2.37), we get that there exists $C$ independent of $n \ge 1$ and $h$ such that

$$\|T_{1,h}^n\|_{L^\infty \to L^\infty} + \|T_{2,h}^n\|_{L^\infty \to L^\infty}. \le Ch^{-3d/2} \tag{2.43}$$

Since $T_h^n$ is bounded by 1 on $L^\infty$, we get from $T_h^n - \Pi_0 = T_{h,1}^n + T_{h,2}^n + T_{h,3}^n$

$$\|T_{3,h}^n\|_{L^\infty \to L^\infty}. \le Ch^{-3d/2} \tag{2.44}$$

Next we use (1.2) to write $T_h = m_h + R_h$ with

$$\begin{aligned} \|m_h\|_{L^\infty \to L^\infty} &\le \gamma < 1, \\ \|R_h\|_{L^2 \to L^\infty} &\le C_0 h^{-d/2}. \end{aligned} \tag{2.45}$$

From this, we deduce that for any $p = 1, 2, \dots$, one has $T_h^p = A_{p,h} + B_{p,h}$, with $A_{1,h} = m_h, B_{1,h} = R_h$ and the recurrence relation $A_{p+1,h} = m_h A_{p,h}, B_{p+1,h} = m_h B_{p,h} + R_h T_h^p$. Thus one gets, since $T_h^p$ is bounded by 1 on $L^2$,

$$\begin{aligned} \|A_{p,h}\|_{L^\infty \to L^\infty} &\le \gamma^p, \\ \|B_{p,h}\|_{L^2 \to L^\infty} &\le C_0 h^{-d/2}(1 + \gamma + \dots + \gamma^p) \le C_0 h^{-d/2}/(1-\gamma). \end{aligned} \tag{2.46}$$

Let $\theta = 1 - \delta_0 < 1$ so that $\|T_{3,h}\|_{L^2 \to L^2} \le \theta$. Then one has

$$\|T_{3,h}^n\|_{L^\infty \to L^2} \le \|T_{3,h}^n\|_{L^2 \to L^2} \le \theta^n,$$

and for $n \ge 1$, $p \ge 1$, one gets, using (2.46) and (2.44),

$$\begin{aligned} \|T_{3,h}^{p+n}\|_{L^\infty \to L^\infty} &= \|T_h^p T_{3,h}^n\|_{L^\infty \to L^\infty} \\ &\le \|A_{p,h} T_{3,h}^n\|_{L^\infty \to L^\infty} + \|B_{p,h} T_{3,h}^n\|_{L^\infty \to L^\infty} \\ &\le Ch^{-3d/2}\gamma^p + C_0 h^{-d/2}\theta^n/(1-\gamma). \end{aligned} \tag{2.47}$$

Thus we get, for some $C > 0$, $\mu > 0$,

$$\|T_{3,h}^n\|_{L^\infty \to L^\infty} \le Ce^{-\mu n}, \qquad \forall h, \quad \forall n \ge 1/h, \tag{2.48}$$

and thus the contribution of $T_{3,h}^n$ is far smaller than the bound we have to prove in (2.40).

Next, for the contribution of $T_{2,h}^n$, we just write, since there are at most $Ch^{-d}$ eigenvalues $\lambda_{j,h}$ and using the bound (2.37),

$$\begin{aligned} T_{h,2}^n(x,y) &= \sum_{h^{-\alpha} < \lambda_{j,h} \le h^{-2}\delta_0} (1-h^2\lambda_{j,h})^n e_{j,h}(x) e_{j,h}(y), \\ \|T_{2,h}^n\|_{L^\infty \to L^\infty} &\le Ch^{-3d/2}(1-h^{2-\alpha})^n. \end{aligned} \tag{2.49}$$

Thus we get for some $C_\alpha > 0$,

$$\|T_{2,h}^n\|_{L^\infty \to L^\infty} \le C_\alpha e^{-\frac{nh^{2-\alpha}}{2}}, \qquad \forall h, \quad \forall n \ge h^{-2+\alpha/2}, \tag{2.50}$$

and thus this contribution is still neglectible for $h \in ]0, h_0]$ for $h_0$ small. It remains to study the contribution of $T_{h,1}^n$.

Let $E_\alpha$ be the (finite dimensional) subspace of $L^2(\rho)$ spanned by the eigenvectors $e_{j,h}, \lambda_{j,h} \le h^{-\alpha}$. By Lemma 2.3, one has $\dim(E_\alpha) \le Ch^{-d\alpha/2}$. We next prove a Sobolev-type inequality for the form $\mathcal{E}_{h,\rho}$. For background on Sobolev and the following Nash inequality, see [DSC96], [SC97].

**Lemma 2.4.** *There exist $\alpha > 0$, $p > 2$ and $C$ independent of $h$ such that for all $u \in E_\alpha$, the following inequality holds true:*

$$\|u\|_{L^p}^2 \le Ch^{-2}\left(\mathcal{E}_{h,\rho}(u) + h^2\|u\|_{L^2}^2\right). \tag{2.51}$$

*Proof.* Clearly, one has for $u = \sum_{\lambda_{1,h} \le \lambda_{j,h} \le h^{-\alpha}} a_j e_{j,h} \in E_\alpha$,

$$\mathcal{E}_{h,\rho}(u) + h^2\|u\|_{L^2}^2 = \sum_{\lambda_{1,h} \le \lambda_{j,h} \le h^{-\alpha}} h^2(1 + \lambda_{j,h})|a_j|^2.$$

Take $u \in E_\alpha$ such that $h^{-2}(\mathcal{E}_{h,\rho}(u) + h^2\|u\|_{L^2}^2) \le 1$. Then by (2.21), one has $h^{-2}\mathcal{E}_h(E(u)) \le C_0$. Let $\psi(t) \in C_0^\infty(\mathbb{R})$ be equal to 1 near $t = 0$, and for $v(x) = \sum_{k \in \mathbb{Z}^d} c_k(v)e^{2i\pi kx/A}$, set

$$v = v_L + v_H, \qquad v_L(x) = \sum_{k \in \mathbb{Z}^d} \psi(h|k|)c_k(v)e^{2i\pi kx/A}. \tag{2.52}$$

Then $v = v_L + v_H$ is a decomposition of the extension $v = E(u)$ in low frequencies ($v_L$) and high frequencies ($v_H$). One has $v_L(x) = \int_{\mathbb{R}^d} h^{-d}\theta(\frac{x-y}{h})v(y)dy$, where $\theta$ is the function in the Schwartz space defined by $\hat{\theta}(2\pi z/A) = \psi(|z|)$. Hence, the map $v \mapsto v_L$ is bounded uniformly in $h$ on all the spaces $L^q$ for $1 \le q \le \infty$. Then, from (2.13) we get

$$\|v_L\|_{H^1(B)} \le C. \tag{2.53}$$

Thus, with $u_L = v_L|_\Omega$ and $u_H = v_H|_\Omega$, we get $\|u_L\|_{H^1(\Omega)} \le C$ so by Sobolev for $p < \frac{2d}{d-2}$,

$$\|u_L\|_{L^p} \le C. \tag{2.54}$$

One the other hand, one has also by (2.21),

$$h^{-2}\mathcal{E}_h\left(E(e_{j,h})\right) \le C_0(1 + \lambda_{j,h}), \tag{2.55}$$

and this implies, by (2.13),

$$h^{-2}\|E(e_{j,h})_H\|_{L^2}^2 \le C_0(1 + \lambda_{j,h}) \le C_0(1 + h^{-\alpha}). \tag{2.56}$$

Thus for $\alpha \le 1$, we get $\|E(e_{j,h})_H\|_{L^2} \le Ch^{1/2}$. On the other hand, since $\|e_{j,h}\|_{L^\infty} \le Ch^{-d/2}$, using the definition of the low frequency cut-off we get

$$\|E(e_{j,h})_H\|_{L^\infty} \le \|E(e_{j,h})\|_{L^\infty} + \|E(e_{j,h})_L\|_{L^\infty} \le C\|E(e_{j,h})\|_{L^\infty} \le Ch^{-d/2}.$$

By interpolation we can find some $p > 2$ such that

$$\|E(e_{j,h})_H\|_{L^p} \le C_0 h^{1/4}. \tag{2.57}$$

Thus one gets, for $u = \sum_{\lambda_{1,h}\le\lambda_{j,h}\le h^{-\alpha}} a_j e_{j,h} \in E_\alpha$ with $h^{-2}(\mathcal{E}_{h,\rho}(u) + h^2\|u\|^2_{L^2}) \le 1$,

$$\begin{aligned}\|u_H\|_{L^p} &\le \sum_{\lambda_{1,h}\le\lambda_{j,h}\le h^{-\alpha}} |a_j| \|E(e_{j,h})_H\|_{L^p} \\ &\le C_0 h^{1/4} \dim(E_\alpha)^{1/2} \|u\|_{L^2} \le C h^{1/4} h^{-d\alpha/4}.\end{aligned} \tag{2.58}$$

Our lemma follows from (2.54) and (2.58) if one takes $\alpha$ small. Observe that here, the estimate on the number of eigenvalues (i.e., the estimation of the dimension of $E_\alpha$) is crucial. The proof of Lemma 2.4 is complete. □

From Lemma 2.4, using the interpolation inequality $\|u\|^2_{L^2} \le \|u\|^{\frac{p}{p-1}}_{L^p} \|u\|^{\frac{p-2}{p-1}}_{L^1}$, we deduce the Nash inequality, with $1/D = 2 - 4/p > 0$,

$$\|u\|^{2+1/D}_{L^2} \le C h^{-2} \left(\mathcal{E}_{h,\rho}(u) + h^2\|u\|^2_{L^2}\right) \|u\|^{1/D}_{L^1}, \qquad \forall u \in E_\alpha. \tag{2.59}$$

For $\lambda_{j,h} \le h^{-\alpha}$, one has $h^2\lambda_{j,h} \le 1$, and thus for any $u \in E_\alpha$, one gets $\mathcal{E}_{h,\rho}(u) \le \|u\|^2_{L^2} - \|T_h u\|^2_{L^2}$ and thus we get, from (2.59),

$$\|u\|^{2+1/D}_{L^2} \le C h^{-2} \left(\|u\|^2_{L^2} - \|T_h u\|^2_{L^2} + h^2\|u\|^2_{L^2}\right) \|u\|^{1/D}_{L^1}, \qquad \forall u \in E_\alpha. \tag{2.60}$$

From (2.48) and (2.50), and $T^n_h - \Pi_0 = T^n_{h,1} + T^n_{h,2} + T^n_{h,3}$, we get that there exists $C_2$ such that

$$\|T^n_{1,h}\|_{L^\infty\to L^\infty} \le C_2, \qquad \forall h, \quad \forall n \ge h^{-2+\alpha/2}, \tag{2.61}$$

and thus since $T_{1,h}$ is self adjoint on $L^2$,

$$\|T^n_{1,h}\|_{L^1\to L^1} \le C_2, \qquad \forall h, \quad \forall n \ge h^{-2+\alpha/2}. \tag{2.62}$$

Fix $p \simeq h^{-2+\alpha/2}$. Take $g \in L^2$ such that $\|g\|_{L^1} \le 1$ and consider the sequence $c_n$, $n \ge 0$,

$$c_n = \|T^{n+p}_{1,h} g\|^2_{L^2}. \tag{2.63}$$

Then $0 \le c_{n+1} \le c_n$, and from (2.60) and (2.62), we get

$$\begin{aligned} c_n^{1+\frac{1}{2D}} &\le C h^{-2} \left(c_n - c_{n+1} + h^2 c_n\right) \|T^{n+p}_{1,h} g\|^{1/D}_{L^1} \\ &\le C C_2^{1/D} h^{-2} \left(c_n - c_{n+1} + h^2 c_n\right). \end{aligned} \tag{2.64}$$

From this inequality, we deduce that there exist $A \simeq CC_2 \sup_{0\le n\le h^{-2}} (2+n)(1+h^2-(1-\frac{1}{n+2})^{2D})$ which depends only on $C,\ C_2,\ D$, such that for all $0 \le n \le h^{-2}$, one has $c_n \le (\frac{Ah^{-2}}{1+n})^{2D}$, and thus there exist $C_0$ which depends only on $C,\ C_2,\ D$, such that for $N \simeq h^{-2}$, one has $c_N \le C_0$. This implies

$$\|T^{N+p}_{1,h} g\|_{L^2} \le C_0 \|g\|_{L^1}, \tag{2.65}$$

and thus taking adjoints,

$$\|T^{N+p}_{1,h} g\|_{L^\infty} \le C_0 \|g\|_{L^2}, \tag{2.66}$$

and so we get, for any $n$ and with $N + p \simeq h^{-2}$,

$$\|T^{N+p+n}_{1,h} g\|_{L^\infty} \le C_0 (1 - h^2\lambda_{1,h})^n \|g\|_{L^2}. \tag{2.67}$$

And thus for $n \ge h^{-2}$,

$$\|T^n_{1,h}\|_{L^\infty\to L^\infty} \le C_0 e^{-(n-h^{-2})h^2\lambda_{1,h}} = C_0 e^{\lambda_{1,h}} e^{-ngap}, \qquad \forall h, \quad \forall n \ge h^{-2}. \tag{2.68}$$

This concludes the proof of Theorem 1.1.

*Remark* 1. We believe that (2.37) is true with a power of $\Lambda$ instead of a power of $h$ with $\lambda = 1-h^2\Lambda$. We have no proof for this which is why we use a Nash inequality for $T_{1,h}$.

*Remark* 2. The above proof seems to apply for a more general choice of the elementary Markov kernel $h^{-d}\varphi(\frac{x-y}{h})$. Replace $\varphi$ by a positive symmetric measure of total mass 1 with support in the unit ball, and let $T_h$ be the Metropolis algorithm with this data. Assume that one is able to prove that for some $\delta_0 > 0$ one has $\mathrm{Spec}(T_h) \subset [-1+\delta_0, 1]$ for all $h \le h_0$, and that for some power $M$, one has for some $C, c > 0$,

$$T_h^M(x, dy) = \mu_h(x, dy) + Ch^{-d}1_{|x-y|\le ch}\rho(y)dy, \qquad \mu_h(x, dy) \ge 0.$$

Then there exists $\gamma < 1$ such that $\|\mu_h\|_{L^\infty} \le \gamma$. Moreover, the right inequality in (2.21) and (2.37) are still valid for $T_h^M$. Also, the spectral gap of $T_h^M$ is given by formula (1.4) with $T_h^M(x, dy)$ in place of $K_{h,\rho}(x, y)dy$, and therefore the left inequality in (1.6) holds true, and the right one is true, since if $\rho$ is constant, for any $\theta \in C_0^\infty(\Omega)$, one has $u - T_h u \in O(h^2)$.

We shall use these remarks in the study of the hard disc problem, in Section 4.

# 3 A Proof of Theorem 1.2

In this section, we suppose additionally that $\Omega$ is quasi-regular (Definition 2). For a given continuous density $\rho$, using (2.5) and an approximation of $\rho$ in $L^\infty$ by a sequence of smooth densities $\rho_k$ on $\overline{\Omega}$, one sees that the first assertion (1.18) of Theorem 1.2 is a consequence of the second one (1.19). Assume now that $\rho$ is smooth.

**Lemma 3.1.** *Let $\theta \in C^\infty(\overline{\Omega})$ be such that $\sup(\theta) \cap \Gamma_{\mathrm{sing}} = \emptyset$ and $\partial_n\theta|_{\Gamma_{\mathrm{reg}}} = 0$. Then, with $Q_{h,\rho}$ defined in (2.2), $L_\rho$ defined in (1.11),*

$$Q_{h,\rho}(\theta) = h^2 L_\rho(\theta) + r, \qquad \|r\|_{L^2} \in O(h^{5/2}). \tag{3.1}$$

*Proof.* For $\theta \in C^\infty(\overline{\Omega})$ and $x \in \Omega$, we can use the Taylor formula to get

$$\begin{aligned} Q_{h,\rho}(\theta)(x) = \frac{1}{\mathrm{vol}(B_1)} \int_{A(x,h)} &\min\left(1 + h\frac{\nabla\rho(x)}{\rho(x)}.z + O(h^2|z|^2), 1\right) \\ &\left(-h\nabla\theta(x).z - \frac{h^2}{2}\sum_{i,j} z_i z_j \partial_{x_i}\partial_{x_j}\theta(x) + O(h^3|z|^3)\right) dz, \end{aligned} \tag{3.2}$$

with $A(x, h) = \{z \in \mathbb{R}^d, |z| < 1, x + hz \in \Omega\}$. As $A(x, h) = A^+(x, h) \cup A^-(x, h)$, with $A^\pm(x, h) = \{z \in A(x, h), \pm(\rho(x + hz) - \rho(x)) \ge 0\}$, it follows by an easy computation that

$$\begin{aligned} Q_{h,\rho}(\theta)(x) =& -\frac{h}{\mathrm{vol}(B_1)}\nabla\theta(x).\int_{A(x,h)} zdz - \frac{h^2}{2\mathrm{vol}(B_1)}\sum_{i,j=1}^d \partial_{x_i}\partial_{x_j}\theta(x)\int_{A(x,h)} z_i z_j dz \\ &- \frac{h^2}{\mathrm{vol}(B_1)}\int_{A^-(x,h)} \frac{\nabla\rho(x)}{\rho(x)}.z\nabla\theta(x).zdz + r(x) \\ =& f_1(x) + f_2(x) + f_3(x) + r(x), \end{aligned} \tag{3.3}$$

with $\|r\|_{L^\infty(\Omega)} = O(h^3)$. Let $\chi = 1_{d(x,\partial\Omega)<2h}$, then for $j = 2, 3$,

$$\|\chi f_j\|_{L^2(\Omega)} \le \|\chi\|_{L^2(\Omega)}\|f_j\|_{L^\infty}(\Omega) = O(h^{5/2}), \tag{3.4}$$

thanks to the support properties of $\chi$. Moreover, for $x \in \sup(1-\chi)$, $A(x,h) = \{|z| < 1\}$ and the change of variable $z \mapsto -z$ shows that $(1-\chi)f_2 = -(1-\chi)\frac{\alpha_d}{2}h^2\Delta\theta(x)$ thanks to (1.8). Hence,

$$f_2(x) = -\frac{\alpha_d}{2}h^2\Delta\theta(x) + r(x), \tag{3.5}$$

with $\|r\|_{L^2} = O(h^{5/2})$.

To compute $f_3(x)$ for $x \in \sup(1-\chi)$, we first observe that $|f_3(x)| \le Ch^2|\nabla\rho(x)||\nabla\theta(x)|$. We thus get $\|1_{|\nabla\rho|\le h^{1/2}} f_3\|_{L^\infty} \le Ch^{5/2}\|\nabla\theta\|_{L^\infty}$. At a point $x$ where $|\nabla\rho(x)| \ge h^{1/2}$, we may write $z = t\frac{\nabla\rho(x)}{|\nabla\rho(x)|} + z^\perp$, $t = \frac{z.\nabla\rho(x)}{|\nabla\rho(x)|}$ and $z^\perp.\nabla\rho(x) = 0$. In these coordinates, one has $A^-(x,h) = \{|z| < 1, (t, z^\perp), t|\nabla\rho(x)| + O(h(t^2 + |z^\perp|^2)) \le 0\}$. From $|\nabla\rho(x)| \ge h^{1/2}$ we get that the symmetric difference $R$ between $A^-(x,h)$ and $\{t \le 0\}$ satisfies $\mathrm{meas}(R) = O(h^{1/2})$ (the symmetric difference of two sets $A, B$ is $A \cup B \setminus A \cap B$). Therefore

$$1_{|\nabla\rho|\ge h^{1/2}}(1-\chi)f_3(x) = -h^2 1_{|\nabla\rho|\ge h^{1/2}}\frac{(1-\chi)(x)}{\mathrm{vol}(B_1)}\int_{\{|z|<1,\nabla\rho(x).z\le 0\}}\frac{\nabla\rho(x)}{\rho(x)}.z\nabla\theta(x).zdz + r(x), \tag{3.6}$$

with $\|r\|_{L^\infty} = O(h^{5/2})$. Using the change of variable $z \mapsto z - 2z^\perp$, we get

$$1_{|\nabla\rho|\ge h^{1/2}}(1-\chi)f_3(x) = -h^2 1_{|\nabla\rho|\ge h^{1/2}}\frac{\alpha_d}{2}(1-\chi)(x)\frac{\nabla\rho(x)}{\rho(x)}.\nabla\theta(x) + r(x), \tag{3.7}$$

and therefore, using (3.4), we get

$$f_3(x) = -h^2\frac{\alpha_d}{2}\frac{\nabla\rho(x)}{\rho(x)}.\nabla\theta(x) + r(x), \tag{3.8}$$

with $\|r\|_{L^2} = O(h^{5/2})$. It remains to show that $\|f_1\|_{L^2(\Omega)} = O(h^{5/2})$. Using the change of variable $z \mapsto -z$ we easily obtain $(1-\chi)f_1 = 0$. Hence, it suffices to show that $f_1'(x,h) = \chi\int_{A(x,h)} z.\nabla\theta(x)dz$ satisfies $\|f_1'\|_{L^\infty(\Omega)} = O(h)$. As $\Gamma_{\mathrm{sing}}$ is compact and $\sup(\theta) \cap \Gamma_{\mathrm{sing}} = \emptyset$, this is a local problem near any point $x_0$ of the regular part $\Gamma_{\mathrm{reg}}$ of the boundary. Let $\psi$ be a smooth function such that near $x_0 = (0,0)$ one has $\Omega = \{x_d > \psi(x')\}$. For $x$ close to $x_0$ one has

$$A(x,h) = \left\{z \in \mathbb{R}^d, |z| < 1,\ x_d + hz_d > \psi(x' + hz')\right\}. \tag{3.9}$$

Set

$$A_1(x,h) = \left\{z \in \mathbb{R}^d, |z| < 1,\ x_d + hz_d > \psi(x') + h\nabla\psi(x')z'\right\}, \tag{3.10}$$

then the symmetric difference $R$ between $A(x,h)$ and $A_1(x,h)$ satisfies $\mathrm{meas}(R) = O(h)$ uniformly in $x$ close to $x_0$. This yields

$$f_1'(x,h) = \nabla\theta(x).v(x,h) + r(x), \qquad v(x,h) = \int_{A_1(x,h)} zdz, \tag{3.11}$$

with $\|r\|_{L^\infty} = O(h)$. Let $\nu(x)$ be the vector field defined by $\nu(x) = (-\nabla\psi(x'), 1)$. Observe that $v(x,h) = \phi(\frac{\psi(x')-x_d}{h|\nu(x)|})\frac{\nu(x)}{|\nu(x)|}$ with $\phi(a) = \int_{|z|<1, z_1>a} z_1 dz$, vanishes for $\mathrm{dist}(x,\partial\Omega) > Ch$ and that for $x \in \partial\Omega$, $\nu(x)$ is collinear to the unit normal to the boundary $\overrightarrow{n}(x)$. Since $\partial_n\theta|_{\Gamma_{\mathrm{reg}}} = 0$, we thus get $\|f_1'\|_{L^\infty} = O(h)$. The proof of our lemma is complete. $\square$

Let us recall that we denote $1=\nu_0<\nu_1<\cdots<\nu_j<\dots$ the eigenvalues of $L_\rho$ and $m_j$ the associated multiplicities. We introduce the bilinear form

$$a_\rho(u,v)=\frac{\alpha_d}{2}\langle\nabla u,\nabla v\rangle_{L^2(\rho)}+\langle u,v\rangle_{L^2(\rho)}. \tag{3.12}$$

This defines an Hilbertian structure on $H^1(\Omega)$ which is equivalent to the usual one. We write $\|.\|_{H^1_\rho}$ for the norm induced by $a_\rho$. We denote

$$\mathcal{D}_0=\left\{\theta\in C^\infty(\overline{\Omega}),\theta=0\text{ near }\Gamma_{\text{sing}},\partial_n\theta_{|\Gamma_{\text{reg}}}=0\right\}. \tag{3.13}$$

**Lemma 3.2.** *$\mathcal{D}_0$ is dense in $H^1(\Omega)$.*

*Proof.* Let $f\in H^1(\Omega)$ be orthogonal to $\mathcal{D}_0$ for $a_\rho$. Then, it is orthogonal to $C_0^\infty(\Omega)$ so that $(L_\rho+1)f=0$ in the sense of distributions. In particular $-\Delta f\in L^2(\Omega)$. Hence we can use the Green formula (1.14) to get for any $\theta\in\mathcal{D}_0$, since $a_\rho(f,\theta)=0$,

$$\langle\partial_n f,\rho\theta\rangle_{H^{-1/2},H^{1/2}}=0. \tag{3.14}$$

For any $\psi\in C_0^\infty(\Gamma_{\text{reg}})$, using smooth local coordinates we can find $\tilde{\psi}$ in $\mathcal{D}_0$ such that $\tilde{\psi}_{|\partial\Omega}=\psi$. Consequently,

$$\langle\partial_n f,\rho\psi\rangle_{H^{-1/2},H^{1/2}}=\langle\partial_n f,\rho\tilde{\psi}\rangle_{H^{-1/2},H^{1/2}}=0. \tag{3.15}$$

Hence, $\partial_n f_{|\Gamma_{\text{reg}}}=0$. This shows that $\partial_n f_{|\partial\Omega}\in H^{-1/2}$ is supported in $\Gamma_{\text{sing}}$. From (1.16) this implies $\partial_n f_{|\partial\Omega}=0$. This shows that $f\in D(L_\rho)$. As the operator $L_\rho+1$ is strictly positive, this implies $f=0$. The proof of our lemma is complete. □

We are now in position to achieve the proof of Theorem 1.2. We first observe that if $\nu_h\in[0,M]$ and $\psi_h\in L^2(\rho)$ satisfy $\|\psi_h\|_{L^2}=1$, $h^{-2}Q_{h,\rho}\psi_h=\nu_h\psi_h$, then thanks to Lemma 2.2 the family $(\psi_h)_{h\in]0,1]}$ is relatively compact in $L^2(\rho)$ so that we can suppose (extracting a subsequence $h_k$) that $\nu_h\to\nu$ and $\psi_h\to\psi$ in $L^2(\rho)$, $\|\psi\|_{L^2}=1$, and moreover by Lemma 2.2, the limit $\psi$ belongs to $H^1(\rho)$. Given $\theta\in\mathcal{D}_0$, it follows from self-ajointness of $Q_{h,\rho}$ and Lemma 3.1 that

$$0=\left\langle(h^{-2}Q_{h,\rho}-\nu_h)\psi_h,\theta\right\rangle_{L^2(\rho)}=\langle\psi_h,(L_\rho-\nu_h)\theta\rangle_{L^2(\rho)}+O(h^{1/2}). \tag{3.16}$$

Making $h\to0$ we obtain $\langle\psi,(L_\rho-\nu)\theta\rangle_{L^2(\rho)}=0$ for all $\theta\in\mathcal{D}_0$. It follows that $(L_\rho-\nu)\psi=0$ in the distribution sense, and integrating by parts that $\partial_n\psi$ vanishes on $\Gamma_{\text{reg}}$. Since $\psi\in H^1(\rho)$, we get as above using (1.16) that $\partial_n\psi=0$, and it follows that $\psi\in D(L_\rho)$. This shows that $\nu$ is an eigenvalue of $L_\rho$, and thus (1.19) is satisfied. Moreover, by compactness in $L^2$ of the sequence $\psi_h$, one gets that for any $\epsilon>0$ small enough, there exists $h_\epsilon>0$ such that

$$\sharp\text{Spec}(h^{-2}Q_{h,\rho})\cap[\nu_j-\epsilon,\nu_j+\epsilon]\le m_j, \tag{3.17}$$

for $h\in]0,h_\epsilon]$ with $h_\epsilon>0$ small enough. It remains to show that there is equality in (3.17), and we shall proceed by induction on $j$.

Let $\epsilon>0$, small, be given such that for $0\le\nu_j\le M+1$, the intervals $I_j^\epsilon=[\nu_j-\epsilon,\nu_j+\epsilon]$ are disjoint. Let $(\mu_j)_{j\ge0}$ be the increasing sequence of eigenvalues of $h^{-2}Q_{h,\rho}$, $\sigma_N=\sum_{j=1}^N m_j$ and $(e_k)_{k\ge0}$ the eigenfunctions of $L_\rho$ such that for all $k\in\{1+\sigma_N,\dots,\sigma_{N+1}\}$, one has $(L_\rho-\nu_{N+1})e_k=0$. As 0 is a simple eigenvalue of both $L_\rho$ and $Q_{h,\rho}$, we have clearly $\nu_0=\mu_0=0$ and $m_0=1=\sharp\text{Spec}(h^{-2}Q_{h,\rho})\cap[\nu_0-\epsilon,\nu_0+\epsilon]$.

Suppose that for all $n\le N$, $m_n=\sharp\text{Spec}(h^{-2}Q_{h,\rho})\cap[\nu_n-\epsilon,\nu_n+\epsilon]$. Then, one has by (1.19), for $h\le h_\varepsilon$,

$$\mu_{1+\sigma_N}\ge\nu_{N+1}-\epsilon. \tag{3.18}$$

By the min-max principle, if $G$ is a finite dimensional subspace of $H^1$ with $\dim(G) = 1 + \sigma_{N+1}$, one has

$$\mu_{\sigma_{N+1}} \leq \sup_{\psi \in G, \|\psi\|=1} \langle h^{-2} Q_{h,\rho}\psi, \psi\rangle_{L^2(\rho)} \tag{3.19}$$

Thanks to Lemma 3.2, for all $e_k, 0 \leq k \leq \sigma_{N+1}$ and all $\alpha > 0$, there exists $e_{k,\alpha} \in \mathcal{D}_0$ such that $\|e_k - e_{k,\alpha}\|_{H^1_\rho} \leq \alpha$. Let $G_\alpha$ be the vector space spanned by the $e_{k,\alpha}, 0 \leq k \leq \sigma_{N+1}$. For $\alpha$ small enough, one has $\dim(G_\alpha) = 1 + \sigma_{N+1}$. From Lemma 3.1, one has

$$\langle h^{-2} Q_{h,\rho} e_{k,\alpha}, e_{k',\alpha}\rangle_{L^2(\rho)} = \langle L_\rho e_{k,\alpha}, e_{k',\alpha}\rangle_{L^2(\rho)} + O_\alpha(h^{1/2}). \tag{3.20}$$

Since $e_{k,\alpha} \in \mathcal{D}_0$, one has $\langle L_\rho e_{k,\alpha}, e_{k',\alpha}\rangle_{L^2(\rho)} = \frac{\alpha_d}{2}\langle \nabla e_{k,\alpha}, \nabla e_{k',\alpha}\rangle_{L^2_\rho}$ and $\langle \nabla e_{k,\alpha}, \nabla e_{k',\alpha}\rangle_{L^2_\rho} = \langle \nabla e_k, \nabla e_{k'}\rangle_{L^2_\rho} + O(\alpha)$. Therefore, for $\psi \in G_\alpha$, $\|\psi\| = 1$, we get

$$\langle h^{-2} Q_{h,\rho}\psi, \psi\rangle_{L^2(\rho)} \leq \nu_{N+1} + C\alpha + O_\alpha(h^{1/2}). \tag{3.21}$$

Taking $\alpha > 0$ small enough and $h < h_\alpha$, we obtain from (3.19) and (3.21), $\mu_{\sigma_{N+1}} \leq \nu_{N+1} + \epsilon$. Combining this with (3.18) and (3.17), we get $m_{N+1} = \sharp\mathrm{Spec}(h^{-2}Q_{h,\rho}) \cap [\nu_{N+1} - \epsilon, \nu_{N+1} + \epsilon]$. The proof of Theorem 1.2 is complete. $\square$

# 4 Application to Random Placement of Non-Overlapping Balls

In this section, we suppose that $\Omega$ is a bounded, Lipschitz, quasi-regular, connected, open subset of $\mathbb{R}^d$ with $d \geq 2$. Let $N \in \mathbb{N}, N \geq 2$ and $\epsilon > 0$ be given. Let $\mathcal{O}_{N,\epsilon}$ be the open bounded subset of $\mathbb{R}^{Nd}$,

$$\mathcal{O}_{N,\epsilon} = \left\{x = (x_1, \dots, x_N) \in \Omega^N, \forall\, 1 \leq i < j \leq N, |x_i - x_j| > \epsilon\right\}.$$

We introduce the kernel

$$K_h(x, dy) = \frac{1}{N}\sum_{j=1}^N \delta_{x_1} \otimes \dots \otimes \delta_{x_{j-1}} \otimes h^{-d}\varphi\left(\frac{x_j - y_j}{h}\right) dy_j \otimes \delta_{x_{j+1}} \otimes \dots \otimes \delta_{x_N}, \tag{4.1}$$

and the associated Metropolis operator on $L^2(\mathcal{O}_{N,\epsilon})$

$$T_h(u)(x) = m_h(x)u(x) + \int_{\mathcal{O}_{N,\epsilon}} u(y) K_h(x, dy), \tag{4.2}$$

with

$$m_h(x) = 1 - \int_{\mathcal{O}_{N,\epsilon}} K_h(x, dy). \tag{4.3}$$

The operator $T_h$ is Markov and self -adjoint on $L^2(\mathcal{O}_{N,\epsilon})$. The configuration space $\mathcal{O}_{N,\epsilon}$ is the set of $N$ disjoint closed balls of radius $\epsilon/2$ in $\mathbb{R}^d$, with centers at the $x_j \in \Omega$. The topology of this set, and the geometry of its boundary is generally hard to understand, but since $d \geq 2$, $\mathcal{O}_{N,\epsilon}$ is clearly non-void and connected for a given $N$ if $\epsilon$ is small enough. The Metropolis kernel $T_h$ is associated to the following algorithm: at each step, we choose uniformly at random a ball, and we move its center uniformly at random in $\mathbb{R}^d$ in a ball of radius $h$. If the new configuration is in $\mathcal{O}_{N,\epsilon}$, the change is made. Otherwise, the configuration is kept as it started.

In order to study the random walk associated to $T_h$, we will assume that $N$ and $\epsilon$ are such that $N\epsilon$ is small enough. Under this condition, we prove in Proposition 4.1 that the open set $\mathcal{O}_{N,\epsilon}$ is connected, Lipschitz and quasi-regular, and in Proposition 4.4 we prove that the kernel of the iterated operator $T_h^M$ (with $M$ large, but independent of $h$) admits a suitable lower bound, so that we will be able to use Remark 2 at the end of Section 2. The main results are collected together in Theorem 4.6 below.

We define $\Gamma_{\text{reg}}$ and $\Gamma_{\text{sing}}$ the set of regular and singular points of $\partial\mathcal{O}_{N,\epsilon}$ as follows. Denote $\mathbb{N}_N = \{1, \dots, N\}$. For $x \in \overline{\mathcal{O}}_{N,\epsilon}$ set

$$\begin{aligned} R(x) &= \{i \in \mathbb{N}_N,\ x_i \in \partial\Omega\}, \\ S(x) &= \{\tau = (\tau_1, \tau_2) \in \mathbb{N}_N,\ \tau_1 < \tau_2 \text{ and } |x_{\tau_1} - x_{\tau_2}| = \epsilon\}, \\ r(x) &= \sharp R(x), \qquad s(x) = \sharp S(x). \end{aligned} \tag{4.4}$$

The functions $r$ and $s$ are lower semi-continuous and any $x \in \overline{\mathcal{O}}_{N,\epsilon}$ belongs to $\partial\mathcal{O}_{N,\epsilon}$ iff $r(x)+s(x) \geq 1$. Define

$$\begin{aligned} \Gamma_{\text{reg}} = &\left\{x \in \overline{\mathcal{O}}_{N,\epsilon},\ s(x) = 1 \text{ and } r(x) = 0\right\} \\ &\cup \left\{x \in \overline{\mathcal{O}}_{N,\epsilon},\ s(x) = 0,\ R(x) = \{j_0\} \text{ and } x_{j_0} \in \partial\Omega_{\text{reg}}\right\} \end{aligned} \tag{4.5}$$

and $\Gamma_{\text{sing}} = \partial\mathcal{O}_{N,\epsilon} \setminus \Gamma_{\text{reg}}$. Then $\Gamma_{\text{sing}}$ is clearly closed, and the $\Gamma_{\text{reg}}$ is the union of smooth disjoint hypersurfaces in $\mathbb{R}^{Nd}$.

**Proposition 4.1.** *There exists $\alpha > 0$ such that for $N\epsilon \leq \alpha$, the set $\mathcal{O}_{N,\epsilon}$ is connected, Lipschitz and quasi-regular.*

*Remark* 3. Observe that in the above Proposition, the smallness condition on $\epsilon$ is $N\epsilon \leq \alpha$ where $\alpha > 0$ depends only on $\Omega$. The condition $N\epsilon^d \leq c$, which says that the density of the balls is sufficiently small, does not imply that the set $\mathcal{O}_{N,\epsilon}$ has Lipschitz regularity. As an example, if $\Omega = ]0,1[^2$ is the unit square in the plane, then $x = (x_1, \dots, x_N),\ x_j = ((j-1)\epsilon, 0),\ j = 1, \dots, N$, with $\epsilon = \frac{1}{N-1}$ is a configuration point in the boundary $\partial\mathcal{O}_{N,\epsilon}$. However, $\partial\mathcal{O}_{N,\epsilon}$ is not Lipschitz at $x$: otherwise, there would exist $\nu_j = (a_j, b_j)$ such that $(x_1 + t\nu_1, \dots, x_N + t\nu_N) \in \mathcal{O}_{N,\epsilon}$ for $t > 0$ small enough, and this implies $a_1 > 0, a_{j+1} > a_j$ and $a_N < 0$ which is impossible.

*Proof.* For $\nu \in S^{p-1}$, $p \geq 1$ and $\delta \in ]0,1[$, denote

$$\Gamma_\pm(\nu, \delta) = \{\xi \in \mathbb{R}^p,\ \pm\langle\xi, \nu\rangle > (1-\delta)|\xi|,\ |\langle\xi, \nu\rangle| < \delta\}. \tag{4.6}$$

We remark [AF03] that an open set $\mathcal{O} \subset \mathbb{R}^p$ is Lipschitz if and only if it satisfies the cone property: $\forall a \in \partial\mathcal{O}, \exists\delta > 0, \exists\nu_a \in S^{p-1}, \forall b \in B(a,\delta) \cap \partial\mathcal{O}$ we have

$$b + \Gamma_+(\nu_a, \delta) \subset \mathcal{O} \quad \text{and} \quad b + \Gamma_-(\nu_a, \delta) \subset \mathbb{R}^p \setminus \overline{\mathcal{O}}. \tag{4.7}$$

Let us first show that $\mathcal{O}_{N,\epsilon}$ is connected for $N\epsilon$ small. For $x \in \mathcal{O}_{N,\epsilon}$ define

$$I(x) = \inf_{i \neq j} |x_i - x_j|. \tag{4.8}$$

Then $I(x) > \epsilon$ and we have the following lemma.

**Lemma 4.2.** *There exists $\alpha_0 > 0$ such that for any $N \in \mathbb{N}, \epsilon > 0$ with $N\epsilon \leq \alpha_0$, there exists $\delta_{N,\epsilon} > 0$ such that for any $x \in \mathcal{O}_{N,\epsilon}$ with $I(x) < \alpha_0/N$, there exists a continuous path $\gamma : [0,1] \to \mathcal{O}_{N,\epsilon}$ such that $\gamma(0) = x$ and $I(\gamma(1)) \geq I(x) + \delta_{N,\epsilon}$.*

*Proof.* As $\Omega$ is bounded and Lipschitz, a compactness argument shows that there exists $\delta_0 > 0, r_0 > 0$ such that

$$\begin{aligned}
&\forall x_0 \in \overline{\Omega}, \exists \nu \in S^{d-1}, \forall x \in B(x_0, r_0) \cap \overline{\Omega}, \qquad x + \Gamma_+(\nu, \delta_0) \subset \Omega \\
&\forall x_0 \in \partial\Omega, \exists \nu \in S^{d-1}, \forall x \in B(x_0, r_0) \cap \partial\Omega, \qquad x + \Gamma_-(\nu, \delta_0) \subset \mathbb{R}^d \setminus \overline{\Omega}.
\end{aligned} \tag{4.9}$$

Let $\alpha_0 < \min(\delta_0, r_0)/100$. For $K \in \mathbb{N}^*$ denote $\delta_K = \alpha_0/K^3$, $\rho_K = 10\alpha_0/K^2$. Observe that it suffices to show the following statement:

$$\begin{aligned}
\forall K \in \mathbb{N}^*, \forall \epsilon \in ]0, \alpha_0/K], \forall N \in \mathbb{N}_K, \forall x \in \mathcal{O}_{N,\epsilon} \text{ s.t. } I(x) < \alpha_0/K, \\
\exists \gamma \in C([0,1], \mathcal{O}_{N,\epsilon}), \text{ s.t.} \\
\gamma(0) = x, \quad I(\gamma(1)) \geq I(x) + \delta_K \quad \text{and} \quad \forall t \in [0,1], \ |x - \gamma(t)|_\infty \leq N\rho_K
\end{aligned} \tag{4.10}$$

Let $K \geq 1$ and $0 < \epsilon < \alpha_0/K$. We proceed by induction on $N \in \mathbb{N}_K$. (Recall that $\mathbb{N}_K = \{0, 1, \ldots, K\}$.) In the case $N = 1$, there is nothing to show. Suppose that the above property holds true at rank $N-1$ and let $x \in \mathcal{O}_{N,\epsilon}$ be such that $I(x) < \alpha_0/K$ (this is possible since $\epsilon < \alpha_0/K$). Introduce the equivalence relation on $\mathbb{N}_N$ defined by $i \simeq_x j$ iff $x_i$ and $x_j$ can be connected by a path lying in $\cup_{k \in \mathbb{N}_N} \overline{B}(x_k, 40\alpha_0/K)$ and denote by $c(x)$ the number of equivalence class.

Suppose that $c(x) \geq 2$. Then there exists a partition $\mathbb{N}_N = I \cup J$, such that $N_I = \sharp I \geq 1$, $N_J = \sharp J \geq 1$ and for all $i \in I$, $j \in J$, $|x_i - x_j| > 40\alpha_0/K$. By induction, there exists a path $\gamma_I : [0,1] \to \Omega^{N_I} \cap \{(x_i)_{i \in I}, \ \forall i \neq j, |x_i - x_j| > \epsilon\}$ such that $\gamma_I(0) = (x_i)_{i \in I}$, $I(\gamma_I(1)) \geq I(\gamma_I(0)) + \delta_K$ and $|\gamma_I(0) - \gamma_I(t)|_\infty < N_I \rho_K$. The same construction for the set $J$ provides a path $\gamma_J$ with the same properties. Define the path $\tilde{\gamma}$ on $[0,1]$ by $(\tilde{\gamma}(t))_i = (\gamma_I(t))_i$ for $i \in I$ and $(\tilde{\gamma}(t))_j = (\gamma_J(t))_j$ for $j \in J$. Since $40\alpha_0/K - (N_I + N_J)\rho_K > \alpha_0/K + \delta_K > \epsilon$, $\tilde{\gamma}$ has values in $\mathcal{O}_{N,\epsilon}$ and we have $I(\tilde{\gamma}(1)) \geq I(x) + \delta_K$ as well as

$$|x - \gamma(t)|_\infty < \max(N_I, N_J)\rho_K \leq (N-1)\rho_K. \tag{4.11}$$

Suppose now that there is only one equivalence class. Then for all $k \in \mathbb{N}_N$, $|x_1 - x_k| \leq 40\alpha_0 N/K \leq 40\alpha_0 < r_0$, were $r_0$ is defined in (4.9). In particular, there exists $\nu \in S^{d-1}$ such that for all $y \in B(x_1, 40\alpha_0) \cap \Omega$, $y + \Gamma_+(\nu, \delta_0) \subset \Omega$. On the other hand, we can suppose without loss of generality that

$$\langle x_1, \nu \rangle \leq \cdots \leq \langle x_N, \nu \rangle. \tag{4.12}$$

For $j \in \{1, ..., N\}$ set $a_j = j\rho_K$ and

$$\gamma(t) = (x_1 + ta_1\nu, ..., x_N + ta_N\nu), \quad t \in [0,1] \tag{4.13}$$

Then, one has $|x - \gamma(t)|_\infty \leq \sup a_j = N\rho_K$, $x_j + ta_j\nu \in \Omega$ since $N\rho_K \leq \delta_0$, and for $i < j$

$$\begin{aligned}
|(x_j + ta_j\nu) - (x_i + ta_i\nu)|^2 &= |x_j - x_i|^2 + 2t(a_j - a_i)\langle x_j - x_i, \nu \rangle + t^2|a_j - a_i|^2 \\
&\geq |x_j - x_i|^2 + t^2|a_j - a_i|^2
\end{aligned} \tag{4.14}$$

Thus one has

$$I(\gamma(1))^2 \geq I(x)^2 + \rho_K^2 \geq (I(x) + \delta_K)^2 \tag{4.15}$$

The proof of lemma 4.2 is complete. $\square$

Using this lemma, it is easy to show that $\mathcal{O}_{N,\epsilon}$ is connected for $N\epsilon$ small. For $x \in \mathcal{O}_{N,\epsilon}$, define

$$\mathcal{I}_x = \{y \in \mathcal{O}_{N,\epsilon}, \exists \gamma \in C([0,1], \mathcal{O}_{N,\epsilon}), \gamma(0) = x, \gamma(1) = y\}. \tag{4.16}$$

We first show easily that there exists $y \in \mathcal{I}_x$ such that $I(y) \geq \alpha_0/N$ if $N\epsilon < \alpha_0$. Let $M = \max_{y \in \mathcal{I}_x} I(y)$. As $I$ is a bounded function, $M$ is finite and given $\gamma \in ]0, \delta_{N,\epsilon}/2[$, there exists $y_1 \in \mathcal{I}_x$ such that $I(y_1) \geq M - \gamma$. If $I(y_1) < \alpha_0/N$, Lemma 4.2 shows that there exists $y_2 \in \mathcal{I}_x$ such that $I(y_2) \geq I(y_1) + \delta_{N,\epsilon} > M$ which is impossible. This shows that there exists $y \in \mathcal{I}_x$ such that $I(y) \geq \alpha_0/N$. Now by 4.9, for any $x \in \Omega$, there exists $\nu_x \in S^{d-1}$ such that $x + t\nu_x \in \Omega$ for $t \in [0, \delta_0]$ and $dist(x + t\nu_x, \partial\Omega) \geq t \sin\theta_0$ with $\cos\theta_0 = 1 - \delta_0$. Let $\alpha_1 = \alpha_0 \sin\theta_0/20$. Then for $N\varepsilon \leq \alpha_1$, and $I(y) \geq \alpha_0/N$, $\gamma(t) = (y_1 + t\alpha_0/4N\nu_{y_1}, ..., y_N + t\alpha_0/4N\nu_{y_N})$, $t \in [0,1]$ is a path in $\mathcal{O}_{N,\epsilon}$ and one has with $\gamma(1) = y' = (y'_1, ..., y'_N)$, $I(y') \geq \alpha_0/2N$, and $dist(y'_j, \partial\Omega) > 3\varepsilon$ for all $j$.

Let $\mathcal{C}_{N,\epsilon}$ be the set of $x \in \mathcal{O}_{N,\epsilon}$ such that $I(x) \geq \alpha_0/2N$ and $dist(x_j, \partial\Omega) > 3\varepsilon$ for all $j$. It remains to show that for any $x, y \in \mathcal{C}_{N,\epsilon}$ there exists a continous path $\gamma$ from $x$ to $y$, with values in $\mathcal{O}_{N,\epsilon}$ for $N\epsilon \leq \alpha_1$. Decreasing $\alpha_0$ we may assume $6c_d\alpha_0^d < \mathrm{vol}(\Omega)$ with $c_d = \mathrm{vol}(B(0,1))$. Decreasing $\alpha_1$, we get that for any $x, y \in \mathcal{C}_{N,\epsilon}$ with $N\epsilon \leq \alpha_1$, there exists $z \in \mathcal{C}_{N,\epsilon}$ such that

$$|x_p - z_q| \geq \alpha_0/2N \text{ and } |y_p - z_q| \geq \alpha_0/2N \qquad \forall p, q \in \mathbb{N}_N. \tag{4.17}$$

One can easily choose the $z_j$ by induction, since for any $x, y \in \mathcal{O}_{N,\epsilon}$ and any $z_1, ..., z_l \in \Omega$ with $0 \leq l \leq N-1$ we have $\mathrm{vol}(\cup_{j=1}^N B(x_j, \alpha_0/N) \cup_{j=1}^N B(y_j, \alpha_0/N) \cup_{j=1}^l B(z_j, \alpha_0/N)) \leq 3Nc_d\alpha_0^d N^{-d} < \mathrm{vol}(\Omega)/2 < \mathrm{vol}(\{x \in \Omega, dist(x, \partial\Omega)\} > 3\epsilon)$.

Thus we are reduced to showing that if $y, z \in \mathcal{C}_{N,\epsilon}$ satisfy 4.17, there exists a continuous path $\gamma$ from $y$ to $z$, with values in $\mathcal{O}_{N,\epsilon}$ if $N\epsilon \leq \alpha_1$. We look for a path $\gamma$ of the form $\gamma = \gamma_N \circ \cdots \circ \gamma_1$, where the path $\gamma_j$ moves only the $j$th ball from $y_j$ to $z_j$. Let us explain how to choose $\gamma_j$. As $\Omega$ is connected, there exists an analytic path $\tilde{\gamma}_1$ which connects $y_1$ to $z_1$ in $\Omega$. We have to modify the path $\tilde{\gamma}_1$ in a new path $\gamma_1$ in order that

$$|\gamma_1(t) - y_j| > \epsilon \qquad \forall j \in \{2, \dots, N\}. \tag{4.18}$$

Let $K = \{t \in [0,1], \exists j_0 \in \{2, \dots, N\}, |\tilde{\gamma}_1(t) - y_{j_0}| \leq 2\epsilon\}$. If $K$ is empty, we set $\gamma_1 = \tilde{\gamma}_1$. If $K$ is non empty, since the path $\tilde{\gamma}_1$ is analytic and $I(y) \geq \alpha_0/2N > 4\epsilon$, $K$ is a disjoint union of intervals, $K = [a_1, b_1] \cup ... \cup [a_L, b_L]$ and for any $l \in \{1, ..., L\}$ there exists a unique $j_l$ such that $|\tilde{\gamma}_1(t) - y_{j_l}| \leq 2\epsilon$ for $t \in [a_l, b_l]$. For $t \notin K$ we set $\gamma_1(t) = \tilde{\gamma}_1(t)$ and for $t \in [a_l, b_l]$ we replace $\tilde{\gamma}_1$ by a continuous path $\gamma_1$ connecting $\tilde{\gamma}_1(a_l)$ to $\tilde{\gamma}_1(b_l)$ on the sphere $|x - y_{j_l}| = 2\epsilon$ which is contained in $\Omega$. Then $\gamma_1(t)$ is continuous. Moreover, as $I(y) > 4\epsilon$, for any $j \in \{2, ..., N\}$ and $t \in [0,1]$ we have $|\gamma_1(t) - y_j| \geq 2\epsilon$. In particular, the path $t \in [0,1] \mapsto (\gamma_1(t), y_2, \dots, y_N)$ has values in $\mathcal{O}_{N,\epsilon}$ and connects $y$ and $\tilde{y} := (z_1, y')$. From (4.17) it is clear that $\tilde{y} \in \mathcal{C}_{N,\epsilon}$ and that (4.17) holds true with $y$ replace by $\tilde{y}$. This permits iterating the construction to build a continuous path from $y$ to $z$. Thus $\mathcal{O}_{N,\epsilon}$ is connected for $N\epsilon < \alpha_1$.

Let us now prove that $\partial\mathcal{O}_{N,\epsilon}$ has Lipschitz regularity for $N\epsilon \leq r_0/2$, where $r_0$ is given by 4.9. For a given $\epsilon$, we will prove this fact by induction on $N \in [1, r_0/2\epsilon]$. The case $N = 1$ is obvious since $\partial\Omega$ is Lipschitz. Let $\overline{x} \in \partial\mathcal{O}_{N,\epsilon}$. The equivalence relation $i \simeq j$ iff $\overline{x}_i$ and $\overline{x}_j$ can be connected by a path lying in the union of closed balls of radius $\epsilon/2$, gives us a partition $\{1, \dots, N\} = \cup_{k=1}^r F_k$ such that

$$\begin{aligned} |\overline{x}_i - \overline{x}_j| &> \epsilon \qquad \forall k \neq l, \forall i \in F_k, \forall j \in F_l; \\ |\overline{x}_{n_l} - \overline{x}_{n_{l+1}}| &= \epsilon \qquad \forall k, \forall i \neq j \in F_k, \exists (n_l) \in F_k, 1 \leq l \leq m, n_1 = i, n_m = j. \end{aligned} \tag{4.19}$$

The Cartesien product $\mathcal{O}_1 \times \mathcal{O}_2$ of two bounded Lipschitz open subsets $\mathcal{O}_i \subset \mathbb{R}^{d_i}$ has Lipschitz regularity. Thus, if $r \geq 2$, the induction hypothesis on $N$ shows that $\partial\mathcal{O}_{N,\epsilon}$ has Lipschitz regularity near $\overline{x}$. Thus we may assume $r = 1$, and therefore, for all $i, j$ one has $|\overline{x}_i - \overline{x}_j| \leq \epsilon(N-1) \leq r_0/2$.

Thus there exists $x_0 \in \overline{\Omega}$ such that $\overline{x}_i \in B(x_0, r_0/2)$, and 4.9 gives us a unit vector $\nu$ and $\delta_0 > 0$. We set

$$\overline{\xi}_i = \alpha \overline{x}_i + \nu \tag{4.20}$$

with $\alpha > 0$ small such that $t\overline{\xi}_i \in \Gamma_+(\nu, \delta_0/2)$ for $t > 0$ small. We choose $\beta > 0$, $\rho > 0$, $t_0 > 0$ such that $\beta << \alpha\epsilon^2$, $\beta << \delta_0$, $\rho << \alpha\epsilon^2$, $\rho << r_0$, $t_0|\overline{\xi}_i|^2 << \alpha\epsilon^2$, $t_0 << \delta_0$.

Let $x \in \partial\mathcal{O}_{N,\epsilon}$ be such that $|x_j - \overline{x}_j| \leq \rho$ and $\theta_i \in \mathbb{R}^d$ be such that $|\theta_i| \leq \beta$. Let $\xi_i = \overline{\xi}_i + \theta_i$, and $\xi = (\xi_1, \cdots, \xi_N)$. One has $t\xi_i \in \Gamma_+(\nu, \delta_0)$ for $t \in ]0, t_0]$ and $t\xi_i \in \Gamma_-(\nu, \delta_0)$ for $t \in [-t_0, 0[$. From

$$\langle x_i - x_j, \xi_i - \xi_j \rangle = \langle x_i - x_j, \overline{\xi}_i - \overline{\xi}_j \rangle + O(\beta) = \alpha|\overline{x}_i - \overline{x}_j|^2 + O(\beta + \rho) \tag{4.21}$$

and

$$|(x_i + t\xi_i) - (x_j + t\xi_j)|^2 = |x_i - x_j|^2 + 2t\langle x_i - x_j, \xi_i - \xi_j \rangle + t^2|\xi_i - \xi_j|^2 \tag{4.22}$$

we get that the function $t \in [-t_0, t_0] \mapsto g_{i,j}(t) = |(x_i + t\xi_i) - (x_j + t\xi_j)|^2$ is strictly increasing. Since by 4.9 we have $x_i + t\xi_i \in \Omega$ for $t \in ]0, t_0]$, we get $x + t\xi \in \mathcal{O}_{N,\epsilon}$ for $t \in ]0, t_0]$. It remains to show $x + t\xi \notin \overline{\mathcal{O}}_{N,\epsilon}$ for $t \in [-t_0, 0[$. If there exists two indices $i, j$ such that $|x_i - x_j| = \epsilon$, this follows from $g_{i,j}(t) < \epsilon^2$ for $t < 0$. If there exists one indice $i$ such that $x_i \in \partial\Omega$, this follows from $t\xi_i \in \Gamma_-(\nu, \delta_0)$ and the second line of 4.9 which implies $x_i + t\xi_i \notin \overline{\Omega}$ for $t \in [-t_0, 0[$. Thus $\partial\mathcal{O}_{N,\epsilon}$ is Lipschitz.

Let us finally prove that $\mathcal{O}_{N,\epsilon}$ is quasi-regular. Let $u \in H^{-1/2}(\partial\mathcal{O}_{N,\epsilon})$ be supported in $\Gamma_{\text{sing}}$. We have to show that $u$ is identically zero. This is a local problem near any point $\overline{x} \in \Gamma_{\text{sing}}$. Let $\overline{x}$ be such that $s(\overline{x}) = 0$, $R(\overline{x}) = \{j_0\}$ (say $j_0$=1) and $\overline{x}_{j_0} \in \partial\Omega_{\text{sing}}$. Denote $\mathcal{D}_{N,\epsilon} = \{x \in (\mathbb{R}^d)^N,\ |x_i - x_j| > \epsilon,\ \forall 1 \leq i < j \leq N\}$. Let $\chi$ be a cut-off function supported near $\overline{x}$ such that $\sup(\chi) \subset (\mathbb{R}^d \times \Omega^{N-1}) \cap \mathcal{D}_{N,\epsilon}$. Then, for any $\psi \in C_0^\infty(\Omega^{N-1})$ the linear form $u_\psi$ defined on $H^{1/2}(\partial\Omega)$ by

$$\langle u_\psi, f \rangle = \langle \chi u, f(x_1)\psi(x_2, \ldots, x_N) \rangle \tag{4.23}$$

is continuous and supported in $\partial\Omega_{\text{sing}}$. As $\partial\Omega$ is quasi-regular, it follows that $u_\psi$ is equal to zero for all $\psi$ and hence, $\chi u = 0$. Therefore, we can suppose that $u$ is supported in the set $\{r(x) + s(x) \geq 2\}$. Let $v$ be the distribution on $\mathbb{R}^{Nd}$

$$\langle v, \varphi \rangle = \langle u, \varphi|_{\partial\mathcal{O}_{N,\epsilon}} \rangle \tag{4.24}$$

Then $v \in H^{-1}(\mathbb{R}^{Nd})$ and its support is equal to $\sup(u)$. The Sobolev space $H^{-1}$ is preserved by bi-Lipschitz maps. Therefore, if there exists a bi-Lipschitz map $\Phi$ defined near $\overline{x}$ such that locally one has $\Phi(\sup(u)) \subset \{y_1 = y_2 = 0\}$, then $u$ is identically 0 near $\overline{x}$. For $n \in \mathbb{N}$, $n \geq 2$, introduce the following property:

$$(\mathcal{P}_n): \text{ for any } \overline{x} \in \Gamma_{sing} \text{ with } r(\overline{x}) + s(\overline{x}) = n, \text{ we have } u = 0 \text{ near } \overline{x}. \tag{4.25}$$

This property is proved by induction on $n$. By lower semicontinuity of the functions $r$ and $s$, we may assume in the proof that for $x \in \sup(u)$ close to $\overline{x}$, one has $r(x) = r(\overline{x})$ and $s(x) = s(\overline{x})$ and hence $R(x) = R(\overline{x})$ and $S(x) = S(\overline{x})$. Therefore, we are reduced to proving that for $\overline{x} \in \Gamma_{sing}$ with $r(\overline{x}) + s(\overline{x}) \geq 2$ and $u \in H^{-1/2}(\partial\mathcal{O}_{N,\epsilon})$ supported in $R(x) = R(\overline{x})$ and $S(x) = S(\overline{x})$, we have $u = 0$ near $\overline{x}$ .

First assume $r(\overline{x}) = s(\overline{x}) = 1$. Then, we can suppose without losing generality, that $u$ is supported near $\overline{x}$ in $G = (\partial\Omega \times \Omega^{N-1}) \cap \{|x_i - x_2| = \epsilon\}$ for some $i \in \{1, 3, \ldots, N\}$. Denoting $x_i = (x_{i,1}, \ldots, x_{i,d})$, we may assume that near $\overline{x}$, $G$ is given by two equations,

$$\begin{aligned} x_{1,1} &= \alpha(x_1'), \quad x_1' = (x_{1,2}, ..., x_{1,d}) \\ x_{2,k} &= \beta(x_2', x_i), \quad x_2' = (x_{2,1}, ..., x_{2,k-1}, x_{2,k+1}, ..., x_{2,d}). \end{aligned} \tag{4.26}$$

with $\alpha$ Lipschitz and $\beta$ smooth. Then, $\nu(x) = (x_{1,1} - \alpha(x_1'), x_{2,k} - \beta(x_2', x_i), x_1', x_2', x_3, \ldots, x_N)$ defines a local bi-Lipschitz homeomorphism of $\mathbb{R}^{Nd}$ such that $\nu \circ G \subset \{0\}^2 \times \mathbb{R}^{Nd-2}$. Therefore, $\nu_*(v)$ vanishes identically near $\nu(\overline{x})$ and hence $u$ is null near $\overline{x}$.

We may thus assume that $s(\overline{x}) \geq 2$ or $r(\overline{x}) \geq 2$. In the case $s(\overline{x}) \geq 2$, the support of $u$ near $\overline{x}$ is contained in a set $A$ of the form $|x_1 - x_2| = |x_2 - x_3| = \epsilon$ or $|x_1 - x_2| = |x_3 - x_4| = \epsilon$. Since $A$ is a subvariety of $\mathbb{R}^{Nd}$ of codimension 2, we get as above that $u$ is null near $\overline{x}$. In the case $r(\overline{x}) \geq 2$, the support of $u$ near $\overline{x}$ is contained in a set $B$ of the form $\partial\Omega \times \partial\Omega \times \mathbb{R}^{(N-2)d}$ which is near $\overline{x}$ bi-Lipschitz homeomorphic to $(y_1 = y_2 = 0) \times \mathbb{R}^{Nd-2}$, and thus $u$ is null near $\overline{x}$. The proof of Proposition 4.1 is complete. ☐

Define for $j \in \mathbb{N}_N$ the two functions $\pi_j$ from $\mathbb{R}^{Nd}$ to $\mathbb{R}^{Nd}$ and $\sigma_j$ from $\mathbb{R}^d$ to $\mathbb{R}^{Nd}$ by

$$\begin{aligned} \pi_j(x_1, \ldots, x_j, \ldots, x_N) &= (x_1, \ldots, 0, \ldots, x_N), \\ \sigma_j(y) &= (0, \ldots, y, \ldots, 0), \end{aligned} \tag{4.27}$$

so that $x = \pi_j(x) + \sigma_j(x_j)$. The following geometric lemma will be the main ingredient of the proof of Proposition 4.4.

**Lemma 4.3.** *Let $\alpha_0 = r_0/10$ with $r_0$ given by 4.9. For all $N \in \mathbb{N}$ and $\epsilon \in ]0, \alpha_0/N]$, there exists $\delta_{N,\epsilon} > 0$ and a finite covering $(U_l)_l$ of $\overline{\mathcal{O}}_{N,\epsilon}$ such that for all $l$, there exists $j$ and $\nu \in S^{d-1}$ such that*

$$x + \sigma_j(\Gamma_+(\nu, \delta_{N,\epsilon})) \subset \mathcal{O}_{N,\epsilon} \qquad \forall x \in U_l \cap \mathcal{O}_{N,\epsilon}. \tag{4.28}$$

*Proof.* Since $\overline{\mathcal{O}}_{N,\epsilon}$ is compact, we have to prove that for any given $x^0 \in \overline{\mathcal{O}}_{N,\epsilon}$, there exist $r > 0$, $\delta = \delta_{N,\epsilon} > 0$, $j$ and $\nu \in S^{d-1}$ such that (4.28) holds true for $x \in \mathcal{O}_{N,\epsilon} \cap B(x^0, r)$. This means that we can select one ball, and that moving only this ball by a vector in $\Gamma_+(\nu, \delta)$ while keeping the other balls fixed, results in an admissible configuration. We shall proceed by induction on $N \geq 1$. For $N = 1$, this is true since $\Omega$ is Lipschitz. Let $N \geq 2$. If one can write $\{1, \ldots, N\}$ as the disjoint union $I \cup J$ with $\sharp I \geq 1, \sharp J \geq 1$, and

$$|x_i^0 - x_j^0| \geq 5\epsilon \qquad \forall i \in I, \forall j \in J, \tag{4.29}$$

then, by the induction hypothesis, the result is true for some $\delta_{N,\epsilon} \in ]0, 4\epsilon[$. Thus, using the definition of $\alpha_0$, we may assume that all the $x_i^0$ are in a small neighborhood of a given point $y^0 \in \overline{\Omega}$ and $sup_k|x_k^0 - y^0| \leq r_0/2$. By 4.9 there exist $\nu, \delta_0 > 0, r_0 > 0$ such that

$$y \in \overline{\Omega} \quad \text{and} \quad |y - y^0| \leq r_0 \Longrightarrow y + \Gamma_+(\nu, \delta_0) \in \Omega \tag{4.30}$$

It remains to show that there exist $j, r_0' \in ]0, r_0[$, and $\nu', \delta_0' > 0$, with $\Gamma_+(\nu', \delta_0') \subset \Gamma_+(\nu, \delta_0)$, such that for all $x = (x_1, \ldots, x_N) \in \mathcal{O}_{N,\epsilon}$ with $\mathrm{dist}(x, x^0) \leq r_0'$, and all $z \in x_j + \Gamma_+(\nu', \delta_0')$, one has $|z - x_k| > \epsilon$ for all $k \neq j$. This will be a consequence of the following property:

$$\forall \beta > 0, \exists j, \exists \nu' \in S^{d-1} \text{ s.t. } |\nu' - \nu| \leq \beta \quad \text{and} \quad \nu'.(x_j^0 - x_k^0) > 0 \ \forall k \neq j. \tag{4.31}$$

In fact, if (4.31) holds true, first take $\beta$ small enough, such that for all $\nu' \in S^{d-1}$ with $|\nu' - \nu| \leq \beta$ there exists $\delta_0' > 0$ with $\Gamma_+(\nu', \delta_0') \subset \Gamma_+(\nu, \delta_0)$; then (4.31) gives us a pair $\nu', j$ such that $\nu'.(x_j^0 - x_k^0) > 0 \ \forall k \neq j$. For $r_0' > 0, \delta_0' > 0$ small enough, we get for all $\xi \in \Gamma_+(\nu', \delta_0')$ and all $x \in \mathcal{O}_{N,\epsilon}, \mathrm{dist}(x, x^0) \leq r_0'$, that $inf_{k \neq j} \xi.(x_j - x_k) \geq \delta_0'|\xi|$, and thus there exists $t_0$ such that for $t \in [0, t_0]$ and $k \neq j$, the function $t \mapsto |x_k - (x_j + t\xi)|^2$ is strictly increasing for all $x \in \mathcal{O}_{N,\epsilon}, \mathrm{dist}(x, x^0) \leq r_0'$ and all $\xi \in \Gamma_+(\nu', \delta_0')$.

Let us show that (4.31) holds true. If $j \mapsto \nu.x_j^0$ achieve its maximum at a single $j$, then (4.31) is obvious with $\nu = \nu'$. Otherwise, the set $A = \{\nu' \in S^{d-1}, \exists j \neq k, \nu'.(x_j^0 - x_k^0) = 0\}$ is contained in a finite union of equators in the sphere $S^{d-1}$, with $\nu \in A$, and thus (4.31) is still obvious by taking $\nu' \in S^{d-1} \setminus A$ close to $\nu$. The proof of Lemma 4.3 is complete. $\square$

For $k \in \mathbb{N}^*$ denote $B^k = B_{\mathbb{R}^k}(0,1)$ the unit Euclidean ball and $\varphi_k(z) = \frac{1}{\mathrm{vol}(B^k)} 1_{B_k}(z)$.

**Proposition 4.4.** *Let $N, \epsilon$ be given such that Lemma 4.3 holds true. There exists $h_0 > 0, c_0, c_1 > 0$ and $M \in \mathbb{N}^*$ such that for all $h \in ]0, h_0]$, one has*

$$T_h^M(x, dy) = \mu_h(x, dy) + c_0 h^{-Nd} \varphi_{Nd}\left(\frac{x-y}{c_1 h}\right) dy, \tag{4.32}$$

*where for all $x \in \mathcal{O}_{N,\epsilon}$, $\mu_h(x, dy)$ is a positive Borel measure.*

*Proof.* For $x, y \in \mathcal{O}_{N,\epsilon}$, we set $\mathrm{dist}(x,y) = \sup_{1 \leq i \leq N} |x_i - y_i|$. For $N \geq 1$, denote by $K_{h,N}$ the kernel given in (4.1). It is sufficient to prove the following: there exists $h_0 > 0, c_0, c_1 > 0$ and $M(N) \in \mathbb{N}^*$ such that for all $h \in ]0, h_0]$, one has for all nonnegative function $f$,

$$K_{h,N}^{M(N)}(f)(x) \geq c_0 h^{-Nd} \int_{y \in \mathcal{O}_{N,\epsilon}, \mathrm{dist}(y,x) \leq c_1 h} f(y) dy. \tag{4.33}$$

First note that it is sufficient to prove the weaker version: for all $x^0 \in \overline{\mathcal{O}}_{N,\epsilon}$, there exist $M(N, x^0), r = r(x^0) > 0$, $c_0 = c_0(x_0) > 0, c_1 = c_1(x_0) > 0, h_0 = h_0(x_0) > 0$ such that for all $h \in ]0, h_0]$, all $x \in \mathcal{O}_{N,\epsilon}$ and all nonnegative function $f$

$$\mathrm{dist}(x, x^0) \leq 2r \Longrightarrow K_{h,N}^{M(N,x^0)}(f)(x) \geq c_0 h^{-Nd} \int_{y \in \mathcal{O}_{N,\epsilon}, \mathrm{dist}(y,x) \leq c_1 h} f(y) dy. \tag{4.34}$$

Let us verify that (4.34) implies (4.33). Decreasing $r(x_0)$ if necessary, we may assume that any set $\{\mathrm{dist}(x, x^0) \leq 2r(x_0)\}$ is contained in one of the open set $U_l$ of Lemma 4.3. There exists a finite set $F$ such that $\overline{\mathcal{O}}_{N,\epsilon} \subset \cup_{x^0 \in F} \{\mathrm{dist}(x, x^0) \leq r(x_0)\}$. Let $M(N) = \sup_{x^0 \in F} M(N, x_0)$, $c_i' = \min_{x_0 \in F} c_i(x_0)$ and $h_0' = \min_{x_0 \in F} h_0(x_0)$. One has to check that for any $x^0 \in F$ and any $x$ with $\mathrm{dist}(x, x^0) \leq r(x^0)$, the right inequality in (4.34) holds true with $M(N) = M(N, x^0) + n$ in place of $M(N, x^0)$ for some constants $c_0, c_1, h_0$. Let $l$ be such that $\mathrm{dist}(x, x^0) \leq r(x_0)$ implies $x \in U_l$. Let $j$ and $\Gamma_+(\nu, \delta)$ be given by Lemma 4.3. Clearly, if $f$ is nonnegative, one has

$$K_{h,N}^{M(N,x^0)+1}(f)(x) \geq \frac{1}{N} h^{-d} \int_{x + \sigma_j(z) \in \mathcal{O}_{N,\epsilon}} \varphi(z/h) K_{h,N}^{M(N,x^0)}(f)(x + \sigma_j(z)) dz \tag{4.35}$$

For $\mathrm{dist}(x, x^0) \leq 2r(x^0) - c_1' h/2$, and $|z| \leq c_1' h/2, z \in \Gamma_+(\nu, \delta)$, one has $\mathrm{dist}(x + \sigma_j(z), x^0) \leq 2r(x^0)$ and by (4.28), $x + \sigma_j(z) \in \mathcal{O}_{N,\epsilon}$. Moreover, $\mathrm{dist}(y, x) \leq c_1' h/2 \Longrightarrow \mathrm{dist}(y, x + \sigma_j(z)) \leq c_1' h$. From (4.35) and (4.34) we thus get, with a constant $C_\delta$ depending only on the $\delta$ given by Lemma 4.3, and for $h \leq h_0'$,

$$\begin{aligned} \mathrm{dist}(x, x^0) \leq 2r(x^0) - c_1' h/2 &\Longrightarrow K_{h,N}^{M(N,x^0)+1}(f)(x) \\ &\geq \frac{C_\delta}{N} c_0' h^{-Nd} \int_{y \in \mathcal{O}_{N,\epsilon}, \mathrm{dist}(y,x) \leq c_1' h/2} f(y) dy. \end{aligned} \tag{4.36}$$

By induction on $n$, we thus get

$$\begin{aligned} \mathrm{dist}(x, x^0) \leq 2r(x^0) - c_1' h &\Longrightarrow K_{h,N}^{M(N,x^0)+n}(f)(x) \\ &\geq \left(\frac{C_\delta}{N}\right)^n c_0' h^{-Nd} \int_{y \in \mathcal{O}_{N,\epsilon}, \mathrm{dist}(y,x) \leq c_1' \frac{h}{2^n}} f(y) dy. \end{aligned} \tag{4.37}$$

Since $n$ is bounded, we get the desired result with $h_0 = \min(\min_{x^0\in F} r(x^0)/c_1', h_0')$.

To complete the proof, let us show (4.34) by induction on $N$. The case $N = 1$ is obvious. Suppose that (4.34) holds for $N-1$ discs. Let $x^0 \in \overline{\mathcal{O}}_{N,\epsilon}$ be fixed. Thanks to Lemma 4.3, we can suppose that there exists an open neighborhood $U$ of $x^0$, a direction $\nu \in S^{d-1}$ and $\delta > 0$ such that (4.28) holds with $j = 1$. Let us denote $x = (x_1, x')$ and define

$$K_{h,N} = K_{h,N,1} + K_{h,N,>} \tag{4.38}$$

with

$$K_{h,N,1}f(x) = \frac{h^{-d}}{N}\int_{(y_1,x')\in\mathcal{O}_{N,\epsilon}} \varphi\left(\frac{x_1-y_1}{h}\right) f\left(y_1,x'\right)dy_1. \tag{4.39}$$

We also denote $G(\nu,\delta) = \{x_1 \in \Gamma_+(\nu,\delta), |x_1| > \frac{\delta}{2}\}$. Then, we have the following:

**Lemma 4.5.** *For any $\delta' \in ]0,\delta/2]$, there exists $C > 0$, $\alpha > 0$, $h_0 > 0$ and $r_0 > 0$ such that $\forall r \in ]0, r_0]$, $\forall h \in ]0, h_0]$, $\forall x \in U \cap \mathcal{O}_{N,\epsilon}$, $\forall \tilde{x} \in x + h(G(\nu,\delta') \times B(0,r)^{N-1})$ with $\tilde{x}' \in \mathcal{O}_{N-1,\epsilon}$, we have $\tilde{x} \in \mathcal{O}_{N,\epsilon}$ and*

$$K_{h,N,>}f(\tilde{x}) \geq CK_{\alpha h,N-1}\left(f(\tilde{x}_1,.)\right)\left(\tilde{x}'\right), \tag{4.40}$$

*for any nonnegative function $f$. In particular, for all $M \in \mathbb{N}^*$, there exists $C, r_0, h_0, \alpha$ as above such that $\forall x \in U \cap \mathcal{O}_{N,\epsilon}$ and $\forall \tilde{x} \in x + h(G(\nu,\delta') \times B(0,r)^{N-1})$, we have*

$$K^M_{h,N,>}f(\tilde{x}) \geq CK^M_{\alpha h,N-1}\left(f(\tilde{x}_1,.)\right)\left(\tilde{x}'\right). \tag{4.41}$$

*Proof.* Inequality (4.41) is obtained easily from (4.40) by induction on $M$. To prove (4.40), observe that for nonnegative $f$ and $\alpha \in ]0,1[$ we have

$$K_{h,N,>}f(\tilde{x}) \geq \frac{h^{-d}}{N}\sum_{j=2}^{N}\int_{A_{j,\alpha,h}(\tilde{x})} f(\tilde{x}_1,\dots,y_j,\dots,\tilde{x}_N)dy_j, \tag{4.42}$$

with $A_{j,\alpha,h}(\tilde{x}) = \{z \in \Omega,\ |\tilde{x}_j - z| < \alpha h \text{ and } \forall k \neq j,\ |\tilde{x}_k - z| > \epsilon\}$. Let $B_{j,\alpha,h}(\tilde{x}) = \{z \in \Omega,\ |\tilde{x}_j - z| < \alpha h \text{ and } \forall k \neq 1, j,\ |\tilde{x}_k - z| > \epsilon\}$. Then $A_{j,\alpha,h} \subset B_{j,\alpha,h}$ and we claim that for $\alpha, r > 0$ small enough and $\tilde{x} \in x + h(G(\nu,\delta') \times B(0,r)^{N-1})$ with $\tilde{x}' \in \mathcal{O}_{N-1,\epsilon}$, we have $B_{j,\alpha,h}(\tilde{x}) = A_{j,\alpha,h}(\tilde{x})$. Indeed, let $\tilde{x}_1 = x_1 + hu_1$ with $u_1 \in G(\nu,\delta')$ and $\tilde{x}' \in \mathcal{O}_{N-1,\epsilon}$ be such that $|\tilde{x}_j - x_j| < hr$. Then for $z \in B_{j,\alpha,h}(\tilde{x})$,

$$|\tilde{x}_1 - z| = |x_1 - x_j + hv_1|, \tag{4.43}$$

with $v_1 = u_1 + \frac{x_j - \tilde{x}_j}{h} + \frac{\tilde{x}_j - z}{h}$. Taking $\alpha, r$ small enough (w.r.t. $\delta$) it follows that $v_1 \in \Gamma_+(\nu,\delta)$. Consequently, Lemma 4.3 shows that $|\tilde{x}_1 - z| > \epsilon$ and hence $z \in A_{j,\alpha,h}(\tilde{x})$ (the same argument shows that $\tilde{x} \in \mathcal{O}_{N,\epsilon}$). Therefore,

$$\begin{aligned} K_{h,N,>}f(\tilde{x}) &\geq \frac{h^{-d}}{N}\sum_{j=2}^{N}\int_{B_{j,\alpha,h}(\tilde{x})} f(\tilde{x}_1,\dots,y_j,\dots,\tilde{x}_N)dy_j \\ &= \frac{(N-1)\mathrm{vol}(B^d)}{N}K_{\alpha h,N-1}\left(f(\tilde{x}_1,.)\right)\left(\tilde{x}'\right), \end{aligned} \tag{4.44}$$

and the proof of Lemma 4.5 is complete. □

Using this lemma we can complete the proof of (4.34). Let $p \in \mathbb{N}$, $\alpha \in ]0, \alpha_0]$ and $x \in \mathcal{O}_{N,\epsilon}$, then

$$\begin{aligned} K_{h,N}^{p+1} f(x) &\geq K_{h,N,1} K_{h,N,>}^{p} f(x) \\ &\geq \frac{h^{-d}}{N} \int_{(z_1,x') \in \mathcal{O}_{N,\epsilon}, z_1 \in x_1 + hG(\nu,\delta')} K_{h,N,>}^{p} f\left(z_1, x'\right) dz_1 \\ &\geq C \frac{h^{-d}}{N} \int_{(z_1,x') \in \mathcal{O}_{N,\epsilon}, z_1 \in x_1 + hG(\nu,\delta')} K_{\alpha h,N-1}^{p} \left(f(z_1,.)\right) \left(x'\right) dz_1, \end{aligned} \tag{4.45}$$

thanks to Lemma 4.5. From the induction hypothesis we can choose $p \in \mathbb{N}$ so that

$$K_{h,N}^{p+1} f(x) \geq C h^{-Nd} \int_{(z_1,x') \in \mathcal{O}_{N,\epsilon}, z_1 \in x_1 + hG(\nu,\delta')} \int_{|x'-y'| < \alpha h, y' \in \mathcal{O}_{N-1,\epsilon}} f\left(z_1, y'\right) dy' dz_1 \tag{4.46}$$

Hence, for any $\beta \in ]0, 1]$ we get

$$K_{h,N}^{p+2} f(x) \geq K_{h,N}^{p+1} K_{h,N,1} f(x) \geq C h^{-Nd} \int_{D_{\alpha,\beta,h}(x)} f\left(y_1, y'\right) \gamma_h(x, y_1) dy_1 dy', \tag{4.47}$$

with

$$D_{\alpha,\beta,h}(x) = \left\{ y \in \mathcal{O}_{N,\epsilon},\ |x' - y'| < \alpha h, |x_1 - y_1| < \beta h \right\} \tag{4.48}$$

and

$$\gamma_h(x, y_1) = h^{-d} \int_{(z_1,x') \in \mathcal{O}_{N,\epsilon}, z_1 \in x_1 + hG(\nu,\delta')} 1_{|z_1 - y_1| < h} dz_1. \tag{4.49}$$

We have to show that $\gamma_h$ is bounded from below by a positive constant, uniformly with respect to $(x, y_1)$ when $|x_1 - y_1| < \beta h$. For $z_1 \in x_1 + hG(\nu, \delta')$, one has $|z_1 - y_1| \leq |z_1 - x_1| + |x_1 - y_1| \leq h\delta' + h\beta < h$ for $\beta$ and $\delta'$ small. Thus for $|x_1 - y_1| < \beta h$ one has

$$\gamma_h(x, y_1) = h^{-d} \int_{(z_1,x') \in \mathcal{O}_{N,\epsilon}, z_1 \in x_1 + hG(\nu,\delta')} dz_1 = \int_{u \in G(\nu,\delta')} 1_{(x_1 + hu, x') \in \mathcal{O}_{N,\epsilon}} du. \tag{4.50}$$

Using Lemma 4.3 again, we get for $|x_1 - y_1| < \beta h$

$$\gamma_h(x, y_1) = \int_{u \in G(\nu,\delta')} du = C_0 > 0. \tag{4.51}$$

Plugging this lower bound into (4.47), gives

$$K_{h,N}^{p+2} \geq C h^{-Nd} \int_{D_{\alpha,\beta,h}(x)} f(y) dy, \tag{4.52}$$

and the proof of (4.34) is complete. This completes the proof of Proposition 4.4. □

By Proposition 4.1, we can consider the Neumann Laplacian $|\Delta|_N$ on $\mathcal{O}_{N,\epsilon}$ defined by

$$\begin{aligned} |\Delta|_N &= -\frac{\alpha_d}{2N} \Delta, \\ D(|\Delta|_N) &= \left\{ u \in H^1(\mathcal{O}_{N,\epsilon}),\ -\Delta u \in L^2(\mathcal{O}_{N,\epsilon}),\ \partial_n u|_{\partial \mathcal{O}_{N,\epsilon}} = 0 \right\}. \end{aligned} \tag{4.53}$$

We still denote $0 = \nu_0 < \nu_1 < \nu_2 < \dots$ the spectrum of $|\Delta|_N$ and $m_j$ the multiplicity of $\nu_j$. Our main result is the following.

**Theorem 4.6.** *Let $N \geq 2$ be fixed. Let $\epsilon > 0$ be small enough such that Proposition 4.1 and Proposition 4.4 hold true. Let $R > 0$ be given and $\beta > 0$ such that the spectrum $\nu_j$ of the Neumann Laplacian (4.53) satisfies $\nu_{j+1} - \nu_j > 2\beta$ for all $j$ such that $\nu_{j+2} \leq R$.*

*There exists $h_0 > 0$, $\delta_0 \in ]0, 1/2[$ and constants $C_i > 0$ such that for any $h \in ]0, h_0]$, the following hold true:*

*i) The spectrum of $T_h$ is a subset of $[-1 + \delta_0, 1]$, 1 is a simple eigenvalue of $T_h$, and $\mathrm{Spec}(T_h) \cap [1 - \delta_0, 1]$ is discrete. Moreover,*

$$\begin{aligned} &\mathrm{Spec}\left(\frac{1 - T_h}{h^2}\right) \cap ]0, R] \subset \cup_{j \geq 1} [\nu_j - \beta, \nu_j + \beta]; \\ &\sharp\mathrm{Spec}\left(\frac{1 - T_h}{h^2}\right) \cap [\nu_j - \beta, \nu_j + \beta] = m_j \qquad \forall \nu_j \leq R; \end{aligned} \tag{4.54}$$

*and for any $0 \leq \lambda \leq \delta_0 h^{-2}$, the number of eigenvalues of $T_h$ in $[1 - h^2\lambda, 1]$ (with multiplicity) is bounded by $C_1(1 + \lambda)^{dN/2}$.*

*ii) The spectral gap $g(h)$ satisfies*

$$\lim_{h \to 0^+} h^{-2} g(h) = \nu_1 \tag{4.55}$$

*and the following estimate holds true for all integer $n$:*

$$\sup_{x \in \mathcal{O}_{N,\epsilon}} \|T_h^n(x, dy) - \frac{dy}{\mathrm{vol}(\mathcal{O}_{N,\epsilon})}\|_{TV} \leq C_4 e^{-ng(h)}. \tag{4.56}$$

The rest of this section is devoted to the proof of Theorem 4.6.

Let $\mu_h(x, dy)$ be given by (4.32) and $\mu_h(f)(x) = \int_{\mathcal{O}_{N,\epsilon}} f(y)\mu_h(x, dy)$. Thanks to the positivity of $\mu_h(x, dy)$, using the Markov property of $T_h^M$ and Lipschitz-continuity of the boundary, we get for some $\delta_0' > 0$, independant of $h > 0$, small enough

$$\|\mu_h\|_{L^\infty, L^\infty} \leq 1 - \inf_{x \in \mathcal{O}_{N,\epsilon}} \int_{\mathcal{O}_{N,\epsilon}} c_0 h^{-Nd} \varphi_{Nd}\left(\frac{x - y}{c_1 h}\right) dy < 1 - \delta_0'. \tag{4.57}$$

Since by (4.32) $\mu_h$ is self-adjoint on $L^2(\mathcal{O}_{N,\epsilon})$, we also get

$$\|\mu_h\|_{L^1, L^1} \leq 1 - \delta_0', \tag{4.58}$$

and by interpolation it follows that $\|\mu_h\|_{L^2, L^2} \leq 1 - \delta_0'$. In particular the essential spectrum of $T_h^M$ is contained in $[0, 1 - \delta_0']$ so that $\sigma_{\mathrm{ess}}(T_h) \subset [0, 1 - 2\delta_0]$ with $2\delta_0 = 1 - (1 - \delta_0')^{1/M}$. Thus $\mathrm{Spec}(T_h) \cap [1 - \delta_0, 1]$ is discrete. Let us verify that, decreasing $\delta_0 > 0$, we may also assume

$$\mathrm{Spec}(T_h) \subset [-1 + \delta_0, 1]. \tag{4.59}$$

Thanks to the Markov property of $T_h^M$, to prove this, it suffices to find $M \in 2\mathbb{N} + 1$ such that

$$\int_{\mathcal{O}_{N,\epsilon}} \int_{\mathcal{O}_{N,\epsilon}} (u(x) + u(y))^2 \, T_h^M(x, dy) dx \geq \delta_0 \|u\|_{L^2}^2, \tag{4.60}$$

for any $u \in L^2(\Omega)$. Thanks to the proof of Proposition 4.4, there exists $M \in 2\mathbb{N} + 1$ such that

$$\int_{\mathcal{O}_{N,\epsilon}} \int_{\mathcal{O}_{N,\epsilon}} (u(x) + u(y))^2 \, T_h^M(x, dy) dx \geq c_0 h^{-Nd} \int_{\mathcal{O}_{N,\epsilon} \times \mathcal{O}_{N,\epsilon}} (u(x) + u(y))^2 \, \varphi_{Nd}\left(\frac{x - y}{c_1 h}\right) dx dy. \tag{4.61}$$

Hence, (4.59) follows from (4.61) and (2.7).

Following the strategy of Section 2 we put $\mathcal{O}_{N,\epsilon}$ in a large box $B = ]-A/2, A/2[^{Nd}$ and, thanks to Proposition 4.1, there is an extension map $E : L^2(\mathcal{O}_{N,\epsilon}) \to L^2(B)$ which is also bounded from $H^1(\mathcal{O}_{N,\epsilon})$ into $H^1(B)$. Define

$$\mathcal{E}_{h,k}(u) = \left\langle (1 - T_h^k)u, u \right\rangle_{L^2(\mathcal{O}_{N,\epsilon})}, \tag{4.62}$$

and define $\mathcal{E}_h$ as in Section 2. Moreover, the identities (2.12) and (2.13) remain true with obvious modifications.

**Lemma 4.7.** *There exist $C_0, h_0 > 0$ such that the following holds true for any $h \in ]0, h_0]$ and any $u \in L^2(\mathcal{O}_{N,\epsilon})$:*

$$\mathcal{E}_h(E(u)) \le C_0 \left(\mathcal{E}_{h,M}(u) + h^2\|u\|_{L^2}^2\right). \tag{4.63}$$

*Proof.* Thanks to Lemma 2.2 we have

$$\mathcal{E}_h(E(u)) \le C_0 \left( \int_{\mathcal{O}_{N,\epsilon}\times\mathcal{O}_{N,\epsilon}} (u(x) - u(y))^2 c_0 h^{-Nd} \varphi_{Nd}\left(\frac{x-y}{c_1 h}\right) dydx + h^2\|u\|_{L^2(\mathcal{O}_{N,\epsilon})}\right). \tag{4.64}$$

Combined with (4.32), this shows that

$$\mathcal{E}_h(E(u)) \le C_0 \left( \int_{\mathcal{O}_{N,\epsilon}\times\mathcal{O}_{N,\epsilon}} (u(x) - u(y))^2 T_h^M(x, dy)dx + h^2\|u\|_{L^2(\mathcal{O}_{N,\epsilon})}\right), \tag{4.65}$$

and the proof is complete. □

**Lemma 4.8.** *For any $0 \le \lambda \le \delta_0/h^2$, the number of eigenvalues of $T_h$ in $[1 - h^2\lambda, 1]$ (with multiplicity) is bounded by $C_1(1+\lambda)^{Nd/2}$. Moreover, any eigenfunction $T_h(u) = \lambda u$ with $\lambda \in ]1-\delta_0, 1]$ satisfies the bound*

$$\|u\|_{L^\infty} \le C_2 h^{-Nd/2}\|u\|_{L^2}. \tag{4.66}$$

*Proof.* Suppose that $T_h(u) = \lambda u$ with $\lambda \in [1 - \delta_0, 1]$, then $T_h^M u = \lambda^M u$ and thanks to (4.32), we get

$$\|(\mu_h - \lambda^M)u\|_{L^\infty} = O(h^{-Nd/2}). \tag{4.67}$$

The estimate (4.66) follows from (4.57). Let $\zeta_k(\lambda, h)$ be the number of eigenvalues of $T_h^k$ in the interval $[1 - h^2\lambda, 1]$ for $h^2\lambda < \delta_0$. Thanks to Lemma 4.7, we can mimick the proof of Lemma 2.3 to get

$$\zeta_M(\lambda, h) \le C(1 + \lambda)^{Nd/2}. \tag{4.68}$$

Then from (4.59), one has

$$\zeta_1(\lambda, h) = \zeta_k\left(\frac{1 - (1 - h^2\lambda)^k}{h^2}, h\right). \tag{4.69}$$

Combining (4.68) and (4.69), we easily obtain the announced estimate. The proof of Lemma 4.8 is complete. □

The rest of the proof of Theorem 4.6 follows the strategy of Sections 2 and 3. Using the spectral decomposition (2.41), (2.42) we get easily the estimates (2.48) and (2.50), and it remains to estimate $T_{h,1}^n$. Following the proof of Lemma 2.4, we can find $\alpha > 0$ small enough and $C > 0$ such that the following Nash inequality holds with $1/D = 2 - 4/p > 0$:

$$\|u\|_{L^2}^{2+1/D} \le Ch^{-2}\left(\mathcal{E}_{h,M}(u) + h^2\|u\|_{L^2}^2\right)\|u\|_{L^1}^{1/D}, \qquad \forall u \in E_\alpha. \tag{4.70}$$

From this inequality, we deduce that for $k \geq h^{-2}$,

$$\|T_{1,h}^{kM}\|_{L^\infty,L^\infty} \leq Ce^{-kMg(h)}, \tag{4.71}$$

and this implies for $k \geq h^{-2}$, since the contributions of $T_{2,h}^{kM}, T_{3,h}^{kM}$ are negligible,

$$\|T_h^{kM}\|_{L^\infty,L^\infty} \leq C'e^{-kMg(h)}. \tag{4.72}$$

As $T_h$ is bounded by 1 on $L^\infty$ we can replace $kM$ by $n \geq h^{-2}$ in (4.72) and (4.56) is proved. Assertion (4.55) is an obvious consequence of (4.54). The proof of (4.54) is the same as the one of Theorem 1.2. Thus, the following lemma will end the proof of Theorem 4.6.

**Lemma 4.9.** *Let $\theta \in C^\infty(\overline{\mathcal{O}}_{N,\epsilon})$ be such that* $\sup(\theta) \cap \Gamma_{\text{sing}} = \emptyset$ *and* $\partial_n\theta|_{\Gamma_{\text{reg}}} = 0$. *Then*

$$(1 - T_h)\theta = h^2|\Delta|_N\theta + r, \qquad \|r\|_{L^2} = O(h^{5/2}). \tag{4.73}$$

*Proof.* Let $\theta \in C^\infty(\overline{\mathcal{O}}_{N,\epsilon})$ be such that $\sup(\theta) \cap \Gamma_{\text{sing}} = \emptyset$ and $\partial_n\theta|_{\Gamma_{\text{reg}}} = 0$ and denote $Q_h = 1 - T_h$. Then $Q_h = \frac{1}{N}\sum_{j=1}^N Q_{j,h}$ with

$$Q_{j,h}\theta(x) = \frac{h^{-d}}{\text{vol}(B_1)}\int_\Omega 1_{|x_j-y|<h}\Pi_{k\neq j}1_{|x_k-y|>\epsilon}\left(\theta(x) - \theta\left(\pi_j(x) + \sigma_j(y)\right)\right)dy. \tag{4.74}$$

Let $\chi_0(x) = 1_{\text{dist}(x,\partial\mathcal{O}_{N,\epsilon})<2h}$. The same proof as in Section 3 shows that

$$(1 - \chi_0)Q_{j,h}\theta(x) = -\frac{\alpha_d}{2}h^2\partial_j^2\theta(x) + O_{L^\infty}(h^3), \tag{4.75}$$

so that

$$(1 - \chi_0)Q_h\theta(x) = h^2|\Delta|_N\theta(x) + O_{L^2}(h^3). \tag{4.76}$$

We study $\chi_0 Q_h\theta$. As $\|\chi_0\|_{L^2} = O(h^{1/2})$ it suffices to show that $\|\chi_0 Q_h\theta\|_{L^\infty} = O(h^2)$. On the other hand, by Taylor expansion we have

$$\chi_0 Q_{j,h}\theta(x) = -\frac{h\chi_0(x)}{\text{vol}(B_1)}\int_{|z|<1}\Pi_{k\neq j}1_{|x_j+hz-x_k|>\epsilon}1_{x_j+hz\in\Omega}z.\partial_j\theta(x)dz + O_{L^\infty}(h^2). \tag{4.77}$$

Hence, it suffices to show that

$$v(x) = \chi_0(x)\sum_{j=1}^N\int_{|z|<1}\Pi_{k\neq j}1_{|x_j+hz-x_k|>\epsilon}1_{x_j+hz\in\Omega}z.\partial_j\theta(x)dz \tag{4.78}$$

satisfies $\|v\|_{L^\infty} = O(h)$. Since $\text{dist}(\sup(\theta), \Gamma_{\text{sing}}) > 0$, there exists disjoint compact sets $F_l \subset \{s(x) = 0, R(x) = l\}$, and $F_{i,j} \subset \{r(x) = 0, S(x) = (i,j)\}$ such that

$$\sup(\chi_0\theta) \subset \cup_l \{x, \text{dist}(x, F_l) \leq 4h\} \cup_{i,j} \{x, \text{dist}(x, F_{i,j}) \leq 4h\}.$$

If $x \in \sup(\chi_0\theta)$ is in $\{x, \text{dist}(x, F_1) \leq 4h\}$, then the same parity arguments as in Section 3 show that

$$v(x) = \chi_0(x)\int_{|z|<1,x_1+hz\in\Omega} z.\partial_1\theta(x)dz = O(h). \tag{4.79}$$

If $x \in \sup(\chi_0\theta)$ is in $\{x, \text{dist}(x, F_{1,2}) \leq 4h\}$, then

$$v(x) = \chi_0(x)\int_{|z|<1} z.(\partial_1\theta(x)1_{|x_1+hz-x_2|>\epsilon} + \partial_2\theta(x)1_{|x_2+hz-x_1|>\epsilon})dz \tag{4.80}$$

and the result follows from $(x_1 - x_2).(\partial_1\theta - \partial_2\theta)(x) = 0(h)$ for $\{x, \text{dist}(x, F_{1,2}) \leq 4h\}$, since $\partial_n\theta$ vanishes on the boundary $|x_1 - x_2| = \epsilon$. The proof of Lemma 4.9 is complete. $\square$

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